

NOTES ON THE KIVA-II SOFTWARE AND
CHEMICALLY REACTIVE FLUID MECHANICS

MICHAEL J. HOLST

Numerical Mathematics Group
Computing & Mathematics Research Division
Lawrence Livermore National Laboratory

Livermore, California

NOTES ON THE KIVA-II SOFTWARE AND CHEMICALLY REACTIVE FLUID MECHANICS*

Michael J. Holst
Numerical Mathematics Group
Computing & Mathematics Research Division
Lawrence Livermore National Laboratory

August 1, 1992

Abstract

This report represents a set of working notes regarding the mechanics of chemically reactive fluids with sprays, and their numerical simulation with the KIVA-II software. KIVA-II is a large FORTRAN program developed at Los Alamos National Laboratory for internal combustion engine simulation. It is our hope is that these notes summarize some of the necessary background material in fluid mechanics and combustion, explain the numerical methods currently used in KIVA-II and similar combustion codes, and provide an outline of the overall structure of KIVA-II as a representative combustion program, in order to aid the researcher in the task of implementing KIVA-II or a similar combustion code on a massively parallel computer.

The notes are organized into three parts as follows. In Part I, we give a brief introduction to continuum mechanics, to fluid mechanics, and to the mechanics of chemically reactive fluids with sprays. In Part II, we take a close look at the governing equations of KIVA-II, and discuss the methods employed in the numerical solution of these equations. We draw some conclusions and make some observations in Part III.

*These notes were written while the author was visiting Lawrence Livermore National Laboratory during the summer of 1992, on loan from the Numerical Computing Group in the Department of Computer Science at the University of Illinois, Urbana-Champaign.

Contents

1	Introduction	1
1.1	Numerical simulation of chemically reactive fluids	1
1.2	The KIVA and KIVA-II computer programs	1
1.3	Outline of the report	2
2	Review of Continuum Mechanics	3
2.1	Notation and fundamental theorems	3
2.1.1	Tensor notation	3
2.1.2	The continuum in the Cartesian case	3
2.1.3	The Dubois-Reymond lemma and the divergence theorem	4
2.1.4	General form of a conservation law of continuum mechanics	4
2.1.5	The flux vector	5
2.1.6	The Reynolds transport theorem	6
2.1.7	The material derivative theorem	7
2.2	Conservation of mass	7
2.2.1	Eulerian approach	7
2.2.2	Lagrangian approach	8
2.2.3	Non-conservation form	8
2.3	Conservation of momentum	8
2.3.1	Eulerian approach	8
2.3.2	Lagrangian approach	9
2.3.3	Non-conservation form	9
2.4	Conservation of energy	9
2.4.1	Thermodynamics	9
2.4.2	Eulerian approach	10
2.4.3	Lagrangian approach	10
2.4.4	Non-conservation form	10
2.4.5	An equation for the specific internal energy	11
3	Continuum Mechanics in the Case of Fluids	12
3.1	The stress tensor	12
3.2	The heat flux vector and the force vector	12
3.3	State relations	12
3.4	The Euler equations	13
3.5	The Navier-Stokes equations	13
3.5.1	The compressible case	13
3.5.2	The incompressible case	13
3.6	The governing equations of combustion	14
3.6.1	Chemistry	14
3.6.2	Sprays	14
3.6.3	The modified source and flux terms	14
3.6.4	The combustion equations	15
3.7	Existence and uniqueness of solutions	15
4	The Governing Equations in KIVA-II	16
4.1	The governing equations and unknowns	16
4.1.1	Constants and parameters	17
4.1.2	Turbulence model constants	17
4.2	Source terms due to chemical reactions	18
4.2.1	Equilibrium reactions	18
4.2.2	Kinetic reactions	18
4.2.3	Chemical heat source terms	19

4.3	Source terms due to the spray	19
4.3.1	The spray equation	19
4.3.2	Computing the spray source terms	20
4.4	Boundary conditions	20
5	Discretization of the KIVA-II Equations	21
5.1	Spatial discretization with the ALE method	21
5.1.1	The ALE mesh and mesh parameters	21
5.1.2	The finite volume method	23
5.1.3	Example: the momentum equations	23
5.2	Temporal discretization with variably implicit schemes	23
5.2.1	Theta-methods	24
5.2.2	Example: the momentum equations	24
5.3	The overall time-stepping structure	24
5.3.1	Initialization	24
5.3.2	Phase A – chemistry and spray droplet interactions	27
5.3.3	Phase B – fluid diffusion and droplet velocity calculations	27
5.3.4	Phase C – fluid advection and mesh rezoning	28
6	The Coupled Implicit Phase B Solution in KIVA-II	29
6.1	The SIMPLE algorithm	29
6.2	Predicted pressure by extrapolation	29
6.3	Predicted velocities from the momentum equations	31
6.4	Predicted temperature from the energy equation	31
6.5	Corrected pressure	32
6.5.1	Cell face velocity equation	32
6.5.2	Cell volume equation	32
6.5.3	A linearized equation of state	32
6.6	The conjugate residual method	33
7	Summary and Conclusions	36
7.1	Cray Y-MP and SUN SPARC versions of KIVA-II	36
7.2	Other options for the implicit solves: multilevel methods	37
7.3	Parallel computing and KIVA-II	37
7.4	Parallel multilevel methods	38
	References	39

1 Introduction

This report represents a set of working notes regarding the mechanics of chemically reactive fluids with sprays, and their numerical simulation with the KIVA-II software. KIVA-II is a large FORTRAN program developed at Los Alamos National Laboratory for internal combustion engine simulation. It is our hope is that these notes summarize some of the necessary background material in fluid mechanics and combustion, explain the numerical methods currently used in KIVA-II and similar combustion codes, and provide an outline of the overall structure of KIVA-II as a representative combustion program, in order to aid the researcher in the task of implementing KIVA-II or a similar combustion code on a massively parallel computer.

1.1 Numerical simulation of chemically reactive fluids

The numerical simulation of combustion phenomena is an extremely complex problem, and has only recently been a successful endeavor [6, 32]. The chemical reactions couple together heat and mass transfer, in such a way that turbulence often results. There are essentially three separate (but coupled) systems evolving in the process of combustion: the fluid, which is described by the conservation equations of continuum mechanics; the interaction of the various chemical species making up the fluid, which react both at equilibrium and kinetically; and the interaction between the injected fluid droplets and the reacting fluid. The fully coupled system of governing equations consists of:

- the equations of compressible fluid dynamics
 - equations for conservation of mass, momentum, and energy, plus state equations
- kinetic and equilibrium chemical reactions
 - reaction equations couple to the fluid equations through terms describing increases and decreases of mass densities of various chemical species as they react
 - heat sources are added to the fluid energy equation for kinetic reactions
- spray droplet interactions
 - mass density source terms are added to the fluid equations for species being injected
 - heat source terms are added to the fluid energy equation for droplet interactions
 - a momentum source is also induced by the injected droplets.

A fourth system is sometimes coupled to the systems above in order to capture in some sense the effects of turbulence, referred to as a set of *turbulence modeling equations*.

1.2 The KIVA and KIVA-II computer programs

The KIVA-II computer program (as well as the original KIVA), developed at Los Alamos National Laboratory, was designed to numerically simulate two- and three-dimensional chemically reactive turbulent fluid flows with sprays, as in the simulation of internal combustion engines. KIVA-II numerically integrates the equations of motion of a (possibly turbulent) chemically reactive mixture of fluids, coupled to the equations representing a single-component spray (of fuel, in the case of an internal combustion engine). Just how these systems of equations are coupled in KIVA-II, and how they are integrated numerically, will be one of the topics discussed in this report.

The fundamental papers and reports describing KIVA and KIVA-II are [2, 3, 4, 5, 26], whereas more general background material regarding combustion theory and internal combustion engines can be found in [14, 15, 19]. KIVA-II boasts a number of improvements over the original KIVA, including the use of a coupled implicit diffusion calculation for pressure wave propagation, which is one of the procedures we will be most interested in.

1.3 Outline of the report

The remainder of this report will be presented in three parts, as follows.

In Part I, consisting of §2 and §3, we present a brief introduction to continuum mechanics in general and to fluid mechanics in particular, and get quickly to the heart of the matter: the governing equations of chemically reactive fluids. In order to provide a thorough background for understanding the equations appearing later in the report, in these initial sections we present detailed derivations of the equations from a few basic principles.

In Part II, which includes §4 through §7, we begin with a close look at the governing equations of KIVA-II, which are somewhat more complex than the standard combustion equations with sprays. We then present a discussion of the methods employed for the numerical solution of these equations. In particular, we first take a close look at the ALE (Arbitrary Lagrangian-Eulerian) mesh, and the finite volume method for spatial discretization. This discussion is followed with a description of the temporal discretization by variably implicit methods, in which a time-step is broken into three phases: Phase A, consisting mainly of chemistry and droplet interactions; Phase B, consisting of fluid diffusion and droplet velocity calculations; and Phase C, in which the fluid is convected and the mesh is rezoned. Finally, we focus on the most time-consuming part of the simulation, the Phase B implicit diffusion calculations.

In Part III, consisting of §8, we summarize the report and make some observations.

As a final remark, we have made the point of presenting all derivations and equations in this report in a standard notation which conforms to that used in the reports describing the KIVA-II software (in particular, reference [3]). Therefore, this report may be used to provide background material, so that the non-expert (i.e., the present author) may more easily read and understand the KIVA-II documentation, as well as some of the related literature.

2 Review of Continuum Mechanics

Mathematical formulation of the following three general principles leads to the basic partial differential equations describing the motion of fluids (liquids and gases) and many other physical phenomena that can be regarded as a continuous medium embedded in space:

- I. conservation of mass
- II. conservation of momentum
- III. conservation of energy.

In the following discussion, we review the mathematical formulation of these three principles; first for a general continuous medium, then a fluid, and finally a chemically reactive fluid. In addition to the references cited in the text, the main sources for the material to follow were [7, 16, 25, 30], as well as the introductory chapters of [20].

2.1 Notation and fundamental theorems

The basic assumption of continuum mechanics is the following:

There exists a function $\rho(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}$, the “mass density” of the continuous medium, at all points $\mathbf{x} \in \Omega \subset \mathcal{R}^n$ and all time $t \in [0, \infty)$.

This is in contrast to particle mechanics, in which all mass is concentrated at a number of discrete points. In order to discuss the ramifications of this assumption, we need some notation.

To begin, we denote Euclidean n -space as \mathcal{R}^n , a point of which is denoted $\mathbf{x} = (x_1, \dots, x_n)$, where $x_i \in \mathcal{R}$. The norm in \mathcal{R}^n is defined as $|\mathbf{x}| = (\sum_{i=1}^n x_i^2)^{1/2}$. The set $\Omega \subset \mathcal{R}^n$ denotes a bounded subset of \mathcal{R}^n , and the *boundary* of such a set is denoted $\partial\Omega$.

2.1.1 Tensor notation

Scalar functions (zero order tensors) are denoted as $f(\mathbf{x}) : \Omega \mapsto \mathcal{R}$, vector functions (first order tensors) as $\mathbf{f}(\mathbf{x}) : \Omega \mapsto \mathcal{R}^n$, and matrix functions (second order tensors) as $\mathbf{f}(\mathbf{x}) : \Omega \mapsto \mathbf{L}(\mathcal{R}^n, \mathcal{R}^n)$. In the following, we will employ Einstein’s summation convention whenever an index is repeated in a sum of tensor components; for example, $f_{ij}g_j$ denotes the sum $\sum_{j=1}^n f_{ij}g_j$.

We employ the following notational conventions for tensor products: the dot (scalar) product of two vectors is denoted $\mathbf{f} \cdot \mathbf{g} = f_i g_i$; the dyadic (tensor) product of two vectors is denoted $(\mathbf{f}\mathbf{g})_{ij} = f_i g_j$; and the (vector) products of vectors and second order tensors are denoted $(\mathbf{f} \cdot \mathbf{g})_i = f_{ij} g_j$, and $(\mathbf{g} \cdot \mathbf{f})_i = g_j f_{ji}$. The tensor-tensor (scalar) product is the double sum denoted by $\mathbf{f} : \mathbf{g} = f_{ij} g_{ji}$. Note that *order* matters in this symbolic tensor product notation. For example, for arbitrary vectors \mathbf{u}, \mathbf{v} , and \mathbf{w} , we have that: $\mathbf{u}\mathbf{v} \cdot \mathbf{w} = \mathbf{u}(\mathbf{v} \cdot \mathbf{w}) = (\mathbf{v} \cdot \mathbf{w})\mathbf{u} = (\mathbf{w} \cdot \mathbf{v})\mathbf{u} = \mathbf{w} \cdot \mathbf{v}\mathbf{u} \neq \mathbf{w} \cdot \mathbf{u}\mathbf{v}$, unless $\mathbf{u}\mathbf{v} = \mathbf{v}\mathbf{u}$, which is not true in general.

We will denote single partial differentiation as $D_i f = \partial f / \partial x_i$, and by defining the vector $\nabla = (D_1, \dots, D_n)$, we can define the *gradient*, *divergence*, and *deformation operators* as tensor products: $\text{grad } f = \nabla f = (D_1 f, \dots, D_n f)$, $(\text{grad } \mathbf{f})_{ij} = (\nabla \mathbf{f})_{ij} = D_j f_i$, $\text{div } \mathbf{f} = \nabla \cdot \mathbf{f} = D_i f_i$, and $\text{def } \mathbf{f} = \frac{1}{2}[\nabla \mathbf{f} + (\nabla \mathbf{f})^T]$. Volume integration of a function $f(\mathbf{x})$ over a set Ω is denoted $\int_{\Omega} f \, d\mathbf{x}$, whereas surface integration over the boundary $\partial\Omega$ is denoted $\oint_{\partial\Omega} f \, ds$.

2.1.2 The continuum in the Cartesian case

From this point on, we will be concerned only with the Cartesian case of $n = 3$. The *velocity* of the continuous medium at a point $\mathbf{x} \in \Omega \subset \mathcal{R}^3$ at time $t \in [0, \infty)$ is denoted $\mathbf{u}(\mathbf{x}, t) = (u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t)) = (dx_1/dt, dx_2/dt, dx_3/dt) = d\mathbf{x}/dt$, where $\mathbf{u}(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}^3$. We also assume the existence of the *mass density* ρ of the continuous medium, where $\rho(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}$.

To fully characterize a general continuous medium, in addition to the mass density ρ and medium velocity \mathbf{u} (or the momentum $\rho\mathbf{u}$), we will need to know the energy E (or equivalently the specific internal energy I). Formulating the principles of conservation of mass, momentum, and energy for a general continuous medium

also gives rise to a stress tensor $\bar{\mathbf{T}}$, and a heat flux vector \mathbf{J} . In the case of fluids, $\bar{\mathbf{T}}$ can be represented in terms of the velocity \mathbf{u} and a scalar function p called the *pressure*, whereas the heat flux vector \mathbf{J} can be related to the energy through Fourier's law of heat conduction and an "equation of state". For fluids this leaves six unknowns: ρ , $\mathbf{u} = (u_1, u_2, u_3)$, E , and p . In the following sections, we will develop six equations relating these six unknowns to yield a closed system.

2.1.3 The Dubois-Reymond lemma and the divergence theorem

The following theorem will often be useful to obtain differential forms of conservation laws from the original integral formulations.

Theorem 2.1 (Dubois-Reymond Lemma) *If $F(\mathbf{x}) : \Omega \mapsto \mathcal{R}$ is continuous on all of Ω , and $\int_D F \, d\mathbf{x} = 0$ for every region $D \subset \Omega$, then $F = 0$ in Ω .*

Proof. If F is continuous and $F(\mathbf{x}_1) > 0$ for some \mathbf{x}_1 , then $\exists D_1$ such that $\mathbf{x}_1 \in D_1$ and $F(\mathbf{x}) > 0 \, \forall \mathbf{x} \in D_1$. But then $\int_{D_1} F \, d\mathbf{x} > 0$, giving a contradiction. \square

We note that the Dubois-Reymond lemma is also valid for tensors $\bar{\mathbf{F}}$ of any order. The next theorem, sometimes called the divergence theorem, will be useful for manipulation of conservation law equations, and is used in the formulation of the finite volume discretization method.

Theorem 2.2 (Divergence Theorem) *For any sufficiently smooth function $\mathbf{F}(\mathbf{x}) : \Omega \mapsto \mathcal{R}^3$, if $\mathbf{n}(\mathbf{x}) : \partial\Omega \mapsto \mathcal{R}^3$ is the unit outward normal to $\partial\Omega$, then:*

$$\int_{\Omega} \nabla \cdot \mathbf{F} \, d\mathbf{x} = \oint_{\partial\Omega} \mathbf{n} \cdot \mathbf{F} \, ds. \quad (1)$$

Proof. See for example [29] for a proof using Stoke's theorem (and for a proof of Stoke's theorem), or [10, 23] for direct proofs. \square

We note that the divergence theorem is also valid for tensors $\bar{\mathbf{F}}$ of any order; see for example page 66 of [30] for a discussion. (It must be noted, however, that $\mathbf{n} \cdot \bar{\mathbf{F}} \neq \bar{\mathbf{F}} \cdot \mathbf{n}$ for nonsymmetric tensors $\bar{\mathbf{F}}$ of order higher than one.)

2.1.4 General form of a conservation law of continuum mechanics

For a continuous medium contained in a set $\Omega \subset \mathcal{R}^3$, the intensity of a scalar function W describing a property of the medium in a fixed volume $D \subset \Omega$ with boundary ∂D will vary with time due to *fluxes* and *sources*. Fluxes represent the contributions to the intensity of W from surrounding points of the medium, whereas sources represent external contributions, for example heat sources.

The *flow* or *flux* of any scalar function W defined in Ω is given by a vector function $\mathbf{F}(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}^3$, the *flux vector*, representing the direction and magnitude of the flow of W at each point $\mathbf{x} \in \Omega$, for all time $t \in [0, \infty)$. For the fixed region $D \subset \Omega$, the outward directed flow of W at a point $\mathbf{x} \in \partial D$ and time t is given by $\mathbf{n} \cdot \mathbf{F}$, where $\mathbf{n}(\mathbf{x}, t) : \partial D \times [0, \infty) \mapsto \mathcal{R}^3$ is the unit outward normal vector to ∂D . The *net flux* of W into or out of the fixed region D will then be given by the surface integral

$$\oint_{\partial D} \mathbf{n} \cdot \mathbf{F} \, ds.$$

Surrounding points of the medium may cause flux contributions to W in the fixed region D through the process of *convection* (or *advection*), which refers to the increase or decrease of W due to the motion of the medium (moving at velocity \mathbf{u}), or through the process of *diffusion* (which is independent of the velocity \mathbf{u} of the medium). Therefore, the flux vector \mathbf{F} may be represented as the sum two separate components: a convective component \mathbf{F}_c and a diffusive component \mathbf{F}_d .

If we represent the *sources* with a *source vector* \mathbf{Q} , then \mathbf{Q} may be represented by two components as well: a scalar *volume source* $Q_v(\mathbf{x}, t) : \Omega \mapsto \mathcal{R}$, representing the sources originating in or acting on the volume D , and a vector *surface source* $\mathbf{Q}_s(\mathbf{x}, t) : \Omega \mapsto \mathcal{R}^3$, representing sources entering through or acting

on the boundary ∂D . The net contribution to the intensity of W in D due to the surface source \mathbf{Q}_s will be expressed with a surface integral around the boundary of D as above, whereas the net contribution to W in D due to the volume source Q_v will be simply:

$$\int_D Q_v \, d\mathbf{x}.$$

A general conservation law states that the change per unit time in the intensity of a scalar function W within a fixed volume D , plus the net amount contributed from fluxes \mathbf{F} through the surface ∂D , equals the contributions from the sources Q_v and \mathbf{Q}_s . This statement can be written mathematically as:

$$\frac{d}{dt} \int_D W \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \mathbf{F} \, ds = \int_D Q_v \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \mathbf{Q}_s \, ds. \quad (2)$$

For a vector function \mathbf{W} , the story is the same: the change per unit time in the intensity of \mathbf{W} within a fixed volume D , plus the net amount contributed from fluxes $\bar{\mathbf{F}}$ through the surface ∂D , equals the contributions from the sources \mathbf{Q}_v and $\bar{\mathbf{Q}}_s$. Now, however, since each scalar component function W_i of \mathbf{W} will have a flux vector, a surface source vector, and a scalar volume source, the full vector function \mathbf{W} will have a flux $\bar{\mathbf{F}}(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathbf{L}(\mathcal{R}^3, \mathcal{R}^3)$ and a surface source $\bar{\mathbf{Q}}_s(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathbf{L}(\mathcal{R}^3, \mathcal{R}^3)$ which are *second order Cartesian tensors* (whose columns are the flux and surface source *vectors* for the individual components of \mathbf{W}), and a volume source which is now a *vector function* $\mathbf{Q}_v(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}^3$ (whose components are the *scalar* volume sources for the individual components of \mathbf{W}). The mathematical statement in this case is then:

$$\frac{d}{dt} \int_D \mathbf{W} \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \bar{\mathbf{F}} \, ds = \int_D \mathbf{Q}_v \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \bar{\mathbf{Q}}_s \, ds. \quad (3)$$

In other words, recalling our notational conventions for the product of vectors and second order tensors, equation (3) is just equation (2) taken for each component of \mathbf{W} , written in a compact form.

Equations (2) and (3) are referred to as the *general integral forms of conservation laws* for scalar and vector quantities, respectively. Assuming that the functions involved are sufficiently smooth, we can apply the divergence theorem in each case to obtain:

$$\begin{aligned} \int_D \frac{\partial W}{\partial t} \, d\mathbf{x} + \int_D \nabla \cdot \mathbf{F} \, d\mathbf{x} &= \int_D Q_v \, d\mathbf{x} + \int_D \nabla \cdot \mathbf{Q}_s \, d\mathbf{x} \\ \int_D \frac{\partial \mathbf{W}}{\partial t} \, d\mathbf{x} + \int_D \nabla \cdot \bar{\mathbf{F}} \, d\mathbf{x} &= \int_D \mathbf{Q}_v \, d\mathbf{x} + \int_D \nabla \cdot \bar{\mathbf{Q}}_s \, d\mathbf{x}, \end{aligned}$$

where we have moved the time derivative inside the integral (the integral is *time-independent* since the region D is fixed). If, again, the functions are sufficiently smooth, the Dubois-Reymond lemma can be used to obtain the *general differential forms of conservation laws* for scalar and vector quantities, respectively:

$$\frac{\partial W}{\partial t} + \nabla \cdot \mathbf{F} = Q_v + \nabla \cdot \mathbf{Q}_s \quad (4)$$

$$\frac{\partial \mathbf{W}}{\partial t} + \nabla \cdot \bar{\mathbf{F}} = \mathbf{Q}_v + \nabla \cdot \bar{\mathbf{Q}}_s. \quad (5)$$

Conservation laws written in the above forms are preferable in certain numerical calculations [20, 24], and equations written in these general forms are referred to as being in *conservation form*. *Non-conservation forms* are easily derived from equations in conservation form, as we will see shortly.

2.1.5 The flux vector

The convective component of the flux is the amount of W or \mathbf{W} *transported* with the motion of the continuous medium moving with velocity \mathbf{u} , and is simply:

$$\mathbf{F}_c = W\mathbf{u}, \quad \text{or} \quad \bar{\mathbf{F}}_c = \mathbf{W}\mathbf{u}. \quad (6)$$

The diffusive component of the flux is the amount of W or \mathbf{W} *diffused* to or from surrounding points of the medium, independent of the medium velocity. Empirical evidence suggests that the appropriate form of the diffusive flux vector is given by the *generalized Fick's law* [7, 25]:

$$\mathbf{F}_d = -\kappa\rho\nabla w, \quad \text{or} \quad \bar{\mathbf{F}}_d = -\kappa\rho\nabla\mathbf{w},$$

where $W = \rho w$ and $\mathbf{W} = \rho\mathbf{w}$ are now expressed in terms of unit mass, and the *diffusivity constant* κ varies with the medium. We note that the diffusive component of the flux is not present for some quantities W and \mathbf{W} of interest (such as mass and momentum) in the case of media such as fluids.

Consider now the scalar and vector functions ρw and $\rho\mathbf{w}$. With the above forms for the components of the flux vector, the integral forms of conservation laws in equations (2) and (3) for ρw and $\rho\mathbf{w}$ become:

$$\frac{d}{dt} \int_D \rho w \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot (\rho w \mathbf{u}) \, ds = \oint_{\partial D} \mathbf{n} \cdot (\kappa\rho\nabla w) \, ds + \int_D Q_v \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \mathbf{Q}_s \, ds \quad (7)$$

$$\frac{d}{dt} \int_D \rho\mathbf{w} \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot (\rho\mathbf{w}\mathbf{u}) \, ds = \oint_{\partial D} \mathbf{n} \cdot (\kappa\rho\nabla\mathbf{w}) \, ds + \int_D \mathbf{Q}_v \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \bar{\mathbf{Q}}_s \, ds. \quad (8)$$

Employing the divergence theorem and the Dubois-Reymond lemma then yields the differential forms of conservation laws:

$$\frac{\partial(\rho w)}{\partial t} + \nabla \cdot (\rho w \mathbf{u}) = \nabla \cdot (\kappa\rho\nabla w) + Q_v + \nabla \cdot \mathbf{Q}_s \quad (9)$$

$$\frac{\partial(\rho\mathbf{w})}{\partial t} + \nabla \cdot (\rho\mathbf{w}\mathbf{u}) = \nabla \cdot (\kappa\rho\nabla\mathbf{w}) + \mathbf{Q}_v + \nabla \cdot \bar{\mathbf{Q}}_s. \quad (10)$$

Equations (7) through (10) form the basis of all the conservation laws of continuum mechanics, and in particular, of fluid mechanics.

2.1.6 The Reynolds transport theorem

The above discussion was based on a fixed volume D , referred to as the *Eulerian perspective*. However, there are two common descriptions of continuum mechanics which yield the same equations but from different views:

- Eulerian (*spatial*) view – the viewpoint is at a fixed spatial position
- Lagrangian (*material*) view – the viewpoint moves along with the continuous medium.

As Strang [33] notes: “The fluid is flowing past Euler, who watches Lagrange go by”.

These two viewpoints are related by the following theorem, referred to as either Leibnitz's theorem or the Reynolds transport theorem.

Theorem 2.3 (Reynolds Transport Theorem) *For any sufficiently smooth function $F(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}$ and material region $D(t) \subset \Omega$,*

$$\frac{d}{dt} \int_{D(t)} F \, d\mathbf{x} = \int_{D(t)} \frac{\partial F}{\partial t} \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot (F\mathbf{u}) \, ds. \quad (11)$$

Proof. See for example [7] for a proof. \square

In words, this theorem states that the rate of change of the quantity F in $D(t)$, where $D(t)$ *changes as well*, is equal to the rate at which F changes in an instantaneously coinciding fixed region $D(t)$ at time t plus the flux of F through the boundary of that region. Thus, the rate of change of F at a moving point of the continuous medium is equal to the rate of change of F ignoring the movement, plus the additional change do to the *transport* of F to the new position. The change in F due to the movement of the region $D(t)$ depends of course on the velocity \mathbf{u} , hence the appearance \mathbf{u} in the right-most term of equation (11). Finally, it can be shown that this result also holds for tensors $\bar{\mathbf{F}}$ of any order.

2.1.7 The material derivative theorem

The following theorem will also be useful, and is a consequence of the transport theorem, the divergence theorem, and the principle of conservation of mass, which we discuss in detail in the following section. Although we present it for a scalar function F , it can be shown to hold for tensors $\bar{\mathbf{F}}$ of any order. First, we define the *material derivative* D/Dt as:

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla.$$

Theorem 2.4 (Material Derivative Theorem) *For any sufficiently smooth function $F(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}$ and material region $D(t) \subset \Omega$, assuming conservation of mass, it is true that:*

$$\frac{d}{dt} \int_{D(t)} \rho F \, d\mathbf{x} = \int_{D(t)} \rho \frac{DF}{Dt} \, d\mathbf{x}. \quad (12)$$

Proof. The transport theorem applied to the function (ρF) gives:

$$\frac{d}{dt} \int_{D(t)} \rho F \, d\mathbf{x} = \int_{D(t)} \frac{\partial(\rho F)}{\partial t} \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot (\rho F \mathbf{u}) \, ds.$$

Applying the divergence theorem to the right side of this equation yields:

$$\frac{d}{dt} \int_{D(t)} \rho F \, d\mathbf{x} = \int_{D(t)} \frac{\partial(\rho F)}{\partial t} + \nabla \cdot (\rho F \mathbf{u}) \, d\mathbf{x}.$$

Expanding the derivatives in the right-hand side gives:

$$\frac{d}{dt} \int_{D(t)} \rho F \, d\mathbf{x} = \int_{D(t)} \rho \frac{\partial F}{\partial t} + F \frac{\partial \rho}{\partial t} + F \nabla \cdot (\rho \mathbf{u}) + \rho \mathbf{u} \cdot \nabla F \, d\mathbf{x}.$$

Assuming conservation of mass, $\partial \rho / \partial t + \nabla \cdot (\rho \mathbf{u}) = 0$, our equation becomes:

$$\frac{d}{dt} \int_{D(t)} \rho F \, d\mathbf{x} = \int_{D(t)} \rho \left(\frac{\partial F}{\partial t} + \mathbf{u} \cdot \nabla F \right) \, d\mathbf{x},$$

which when expressed with the material derivative is the same as equation (12). \square

2.2 Conservation of mass

The principle of conservation of mass is simply that mass is neither created nor destroyed. The interpretation of this principle mathematically depends on the viewpoint or frame of reference. It must first be noted that for most continuous media of interest (such as fluids) there is no diffusive component of the mass or momentum flux vectors (see for example [7, 25] for discussions). Also, we assume (for the moment) that there are no mass sources present.

2.2.1 Eulerian approach

In the *Eulerian interpretation*, in the absence of mass source terms and diffusive mass flux, the rate of increase of mass contained in a *fixed region of space* must equal the net convective mass flux into the region. The convective mass flux is the amount of mass density ρ transported by the motion of the medium. As given in equation (6), this is $\mathbf{F}_c = \rho \mathbf{u}$. For a region $D \subset \Omega$, this yields directly from equations (7) and (9) the *integral* and *differential* forms of the *law of conservation of mass* ρ in a continuous medium:

$$\frac{d}{dt} \int_D \rho \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot (\rho \mathbf{u}) \, ds = 0 \quad (13)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (14)$$

2.2.2 Lagrangian approach

In the *Lagrangian interpretation*, the rate of increase (or decrease) of mass ρ contained in a *fixed portion of the continuous medium which moves with the medium* does not change in time. For a fixed portion of the material $D(t) \subset \Omega$, this statement is simply:

$$\frac{d}{dt} \int_{D(t)} \rho \, d\mathbf{x} = 0.$$

From the transport theorem this is:

$$\int_{D(t)} \frac{\partial \rho}{\partial t} \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot (\rho \mathbf{u}) \, d\mathbf{x} = 0.$$

This is exactly equation (13), and the divergence theorem and Dubois-Reymond lemma then yield equation (14) as in the Eulerian approach.

2.2.3 Non-conservation form

Once we have obtained equation (14) through either the Eulerian or Lagrangian approach, we can derive an alternative expression which is in a *non-conservation form*, through use of the material derivative. Since $\nabla \cdot (\rho \mathbf{u}) = \rho \nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \rho$, we can write equation (14) as:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0. \quad (15)$$

2.3 Conservation of momentum

The principle of conservation of momentum is the application of Newton's second law of motion to the continuous medium: the total force on a body equals the rate of change of the total momentum. Again, the mathematical interpretation of this statement depends on our frame of reference. As we noted earlier, there is no diffusive component of momentum flux for most continuous media of interest, such as fluids.

2.3.1 Eulerian approach

In the absence of diffusive momentum flux, in the *Eulerian interpretation*, the rate of change of momentum in a *fixed region of space* plus the net convective flux of momentum through the surface of the region must equal the sum of the forces (or *momentum sources*) acting on the fixed region. Given a force vector per unit mass \mathbf{F} , the momentum volume source vector is $\mathbf{Q}_v = \rho \mathbf{F}$. The convective component of the momentum flux is the amount of momentum $\rho \mathbf{u}$ transported by the motion of the medium and has the form of equation (6), or $\mathbf{F}_c = \rho \mathbf{u} \mathbf{u}$. If in addition we denote the momentum surface source tensor as $\bar{\mathbf{Q}}_s = \bar{\mathbf{T}}$, then we can write down from the general equation forms (8) and (10) the *integral* and *differential* forms of the *law of conservation of momentum* $\rho \mathbf{u}$ directly as:

$$\frac{d}{dt} \int_D \rho \mathbf{u} \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot (\rho \mathbf{u} \mathbf{u}) \, ds = \int_D \rho \mathbf{F} \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot \bar{\mathbf{T}} \, ds \quad (16)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{F} + \nabla \cdot \bar{\mathbf{T}}. \quad (17)$$

The particular forms that \mathbf{F} and $\bar{\mathbf{T}}$ take will depend on the particular type of continuous medium; we will discuss their forms in the special case of fluids shortly. In any case, $\bar{\mathbf{T}}$ is usually taken to be symmetric, $\bar{\mathbf{T}}_{ij} = \bar{\mathbf{T}}_{ji}$, referred to as *conservation of moment of momentum* [25].

2.3.2 Lagrangian approach

In the *Lagrangian interpretation*, as in the case of conservation of mass, the statement of the conservation of momentum has a simpler form:

$$\frac{d}{dt} \int_{D(t)} \rho \mathbf{u} \, d\mathbf{x} = \int_{D(t)} \rho \mathbf{F} \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot \bar{\mathbf{T}} \, ds. \quad (18)$$

The transport theorem then gives:

$$\int_{D(t)} \frac{\partial(\rho \mathbf{u})}{\partial t} + \oint_{\partial D(t)} \mathbf{n} \cdot (\rho \mathbf{u} \mathbf{u}) \, ds = \int_{D(t)} \rho \mathbf{F} \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot \bar{\mathbf{T}} \, ds.$$

The divergence theorem and Dubois-Reymond lemma then give equation (17) as in the Eulerian approach.

2.3.3 Non-conservation form

If we expand the derivatives in equation (17) using the “product rule” (easily verified by employing Einstein’s summation convention) for the divergence of dyadic tensors, $\nabla \cdot (\mathbf{u}\mathbf{v}) = \mathbf{v}\nabla \cdot \mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{v} = \mathbf{v}\nabla \cdot \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{v}$, we obtain:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \frac{\partial \rho}{\partial t} + \mathbf{u} \nabla \cdot (\rho \mathbf{u}) + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \rho \mathbf{F} + \nabla \cdot \bar{\mathbf{T}}.$$

Enforcing conservation of mass $\partial \rho / \partial t + \nabla \cdot (\rho \mathbf{u}) = 0$ in the above equation yields:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \rho \mathbf{F} + \nabla \cdot \bar{\mathbf{T}}.$$

Using the material derivative we have the alternative expression

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \mathbf{F} + \nabla \cdot \bar{\mathbf{T}}, \quad (19)$$

which is now in a *non-conservation form*.

Alternatively, by applying the material derivative theorem to the left-hand side of equation (18), we obtain:

$$\int_{D(t)} \rho \frac{D\mathbf{u}}{Dt} \, d\mathbf{x} = \int_{D(t)} \rho \mathbf{F} \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot \bar{\mathbf{T}} \, ds.$$

An application of the divergence theorem and the Dubois-Reymond lemma then produces equation (19) directly.

2.4 Conservation of energy

The mathematical statement of the principle of conservation of energy is somewhat more complex than the two conservation principles discussed previously, due to certain thermodynamic relationships which must be considered.

2.4.1 Thermodynamics

In continuous media such as fluids, the *total energy per unit mass* E of the medium is the sum of a *specific internal (potential) energy per unit mass* I and the kinetic energy per unit mass:

$$E = I + \frac{\mathbf{u} \cdot \mathbf{u}}{2}.$$

The first law of thermodynamics states that the increase of total energy ρE in a material volume D must equal the work done on the volume plus the heat added to the volume (convected or diffused).

The convective component of the flux vector of the total energy ρE represents the amount of ρE transported by the motion of the medium. As given by equation (6), this is:

$$\mathbf{F}_c = \rho E \mathbf{u}.$$

In contrast to mass and momentum, *the diffusive component of the flux of total energy ρE is present in media such as fluids [7, 25]. We denote this diffusive flux as $\mathbf{F}_d = \mathbf{J}$, referred to as the heat flux vector. The particular form that \mathbf{J} takes for fluids will be discussed shortly.*

The volume component of the energy source Q_v consists of the work done on the volume by unit mass forces \mathbf{F} , with the addition of work represented by possible heat sources q . The rate at which the total force $\rho \mathbf{F}$ does work is the *power* input of $\rho \mathbf{F}$, and is given by $\rho \mathbf{F} \cdot \mathbf{u}$. Therefore, the volume energy source component is given by:

$$Q_v = \rho \mathbf{F} \cdot \mathbf{u} + q.$$

The surface component of the energy source \mathbf{Q}_s is the work done on the volume by internal stress or surface forces $\bar{\mathbf{T}}$, the power input of which are given by:

$$\mathbf{Q}_s = \bar{\mathbf{T}} \cdot \mathbf{u}.$$

2.4.2 Eulerian approach

In the *Eulerian interpretation*, the rate of change of total energy in a *fixed region of space* plus the net (convective and diffusive) flux of energy through the surface of the region must equal the sum of the energy sources acting on the fixed region. Putting this together we can write down the *integral and differential* forms of the *law of conservation of total energy ρE* using the general forms of equations (8) and (10):

$$\frac{d}{dt} \int_D \rho E \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot (\rho E \mathbf{u}) \, ds = - \oint_{\partial D} \mathbf{n} \cdot \mathbf{J} \, ds + \int_D (\rho \mathbf{F} \cdot \mathbf{u} + q) \, d\mathbf{x} + \oint_{\partial D} \mathbf{n} \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}) \, ds \quad (20)$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + \nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}). \quad (21)$$

2.4.3 Lagrangian approach

In the *Lagrangian approach*, the statement of conservation of energy has the simpler form:

$$\frac{d}{dt} \int_{D(t)} \rho E \, d\mathbf{x} = - \oint_{\partial D(t)} \mathbf{n} \cdot \mathbf{J} \, ds + \int_{D(t)} (\rho \mathbf{F} \cdot \mathbf{u} + q) \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}) \, ds. \quad (22)$$

The transport theorem gives:

$$\int_{D(t)} \frac{\partial(\rho E)}{\partial t} + \oint_{\partial D(t)} \mathbf{n} \cdot (\rho E \mathbf{u}) \, ds = - \oint_{\partial D(t)} \mathbf{n} \cdot \mathbf{J} \, ds + \int_{D(t)} (\rho \mathbf{F} \cdot \mathbf{u} + q) \, d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}) \, ds.$$

The divergence theorem and Dubois-Reymond lemma then give equation (21) as in the Eulerian approach.

2.4.4 Non-conservation form

Expanding the derivatives on the right-hand side of equation (21) yields:

$$E \frac{\partial \rho}{\partial t} + \rho \frac{\partial E}{\partial t} + E \nabla \cdot (\rho \mathbf{u}) + \rho \mathbf{u} \cdot \nabla E = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + \nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}).$$

Enforcing conservation of mass $\partial \rho / \partial t + \nabla \cdot (\rho \mathbf{u}) = 0$ in the above equation yields:

$$\rho \frac{\partial E}{\partial t} + \rho \mathbf{u} \cdot \nabla E = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + \nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}).$$

Using the material derivative we have the alternative expression in *non-conservation form*:

$$\rho \frac{DE}{Dt} = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + \nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}). \quad (23)$$

An alternative derivation begins by applying the material derivative theorem to the left-hand side of equation (22), which yields:

$$\int_{D(t)} \rho \frac{DE}{Dt} d\mathbf{x} = - \oint_{\partial D(t)} \mathbf{n} \cdot \mathbf{J} ds + \int_{D(t)} (\rho \mathbf{F} \cdot \mathbf{u} + q) d\mathbf{x} + \oint_{\partial D(t)} \mathbf{n} \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}) ds.$$

Applying first the divergence theorem and then the Dubois-Reymond lemma produces equation (23).

2.4.5 An equation for the specific internal energy

Using the following “product rule” (again, easily verified by employing Einstein’s summation convention) for the divergence of tensor-vector products:

$$\nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}) = (\nabla \cdot \bar{\mathbf{T}}) \cdot \mathbf{u} + \bar{\mathbf{T}} : (\nabla \mathbf{u}),$$

from equation (21) we have the expression:

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + (\nabla \cdot \bar{\mathbf{T}}) \cdot \mathbf{u} + \bar{\mathbf{T}} : (\nabla \mathbf{u}). \quad (24)$$

If we now take the dot product of the momentum equation (19) with \mathbf{u} , the left side of the resulting equation has the form:

$$\begin{aligned} \rho \frac{D\mathbf{u}}{Dt} \cdot \mathbf{u} &= \rho \left(\left[\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] \cdot \mathbf{u} \right) \\ &= \rho \left(\mathbf{u} \cdot \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot [\mathbf{u} \cdot \nabla \mathbf{u}] \right) = \rho \left(\frac{1}{2} \left[\mathbf{u} \cdot \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{u} \right] + \frac{1}{2} \mathbf{u} \cdot [\mathbf{u} \cdot \nabla \mathbf{u} + \nabla \mathbf{u} \cdot \mathbf{u}] \right) \\ &= \rho \left(\frac{\partial}{\partial t} \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] + \mathbf{u} \cdot \nabla \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] \right) = \rho \frac{D}{Dt} \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] = \frac{\partial}{\partial t} \left(\rho \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] \right) + \nabla \cdot \left(\rho \mathbf{u} \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] \right), \end{aligned}$$

where this last equality follows by conservation of mass, as in the derivation of equation (23). This gives an expression for the kinetic energy $[\mathbf{u} \cdot \mathbf{u}]/2$:

$$\frac{\partial}{\partial t} \left(\rho \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] \right) + \nabla \cdot \left(\rho \mathbf{u} \left[\frac{\mathbf{u} \cdot \mathbf{u}}{2} \right] \right) = \rho \mathbf{F} \cdot \mathbf{u} + (\nabla \cdot \bar{\mathbf{T}}) \cdot \mathbf{u}. \quad (25)$$

Since $E = I + [\mathbf{u} \cdot \mathbf{u}]/2$, subtracting equation (25) from equation (24) yields an expression for the internal energy I alone:

$$\frac{\partial(\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\nabla \cdot \mathbf{J} + q + \bar{\mathbf{T}} : (\nabla \mathbf{u}). \quad (26)$$

The associated non-conservation form is easily seen to be:

$$\rho \frac{DI}{Dt} = -\nabla \cdot \mathbf{J} + q + \bar{\mathbf{T}} : (\nabla \mathbf{u}), \quad (27)$$

where we have again employed conservation of mass.

3 Continuum Mechanics in the Case of Fluids

From the previous section, the equations of continuum mechanics representing the conservation of mass, momentum, and energy (in differential, conservation form) are respectively:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (28)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{F} + \nabla \cdot \bar{\mathbf{T}} \quad (29)$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + \nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}). \quad (30)$$

The equivalent non-conservation forms of these equations were seen to be:

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0 \quad (31)$$

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \mathbf{F} + \nabla \cdot \bar{\mathbf{T}} \quad (32)$$

$$\rho \frac{DE}{Dt} = -\nabla \cdot \mathbf{J} + \rho \mathbf{F} \cdot \mathbf{u} + q + \nabla \cdot (\bar{\mathbf{T}} \cdot \mathbf{u}). \quad (33)$$

3.1 The stress tensor

In the case of fluids, the stress tensor $\bar{\mathbf{T}}$ has a particular form. If the fluid is *Newtonian*, then this form is assumed to be [7, 30]

$$\bar{\mathbf{T}} = -p\bar{\mathbf{I}} + \bar{\sigma},$$

where $\bar{\sigma}$ is the *viscous shear stress tensor*, p is a scalar function $p(\mathbf{x}, t) : \Omega \times [0, \infty) \mapsto \mathcal{R}$ called the *pressure*, and $\bar{\mathbf{I}}$ is the unit tensor.

3.2 The heat flux vector and the force vector

Empirical evidence suggests that the heat flux vector \mathbf{J} can be given by *Fourier's law of heat conduction* [7, 25]

$$\mathbf{J} = -K\nabla T,$$

where K is the coefficient of thermal conductivity or diffusivity, and T is the absolute temperature. The force vector \mathbf{F} is often due to gravity, so it is usually denoted as \mathbf{g} .

3.3 State relations

We will discuss below how the viscous stress tensor $\bar{\sigma}$ can be written in terms of the velocity gradients and scalar viscosity coefficients which depend on the fluid state (temperature and pressure). Given that this is the case, we then have the five equations (28)–(30) relating the seven unknowns: ρ , $\mathbf{u} = (u_1, u_2, u_3)$, E (or I), T , and p . An *equation of state* of the form:

$$p = p(\rho, T), \quad (34)$$

representing the nature of the particular fluid involved, is taken to provide a sixth equation relating the unknowns. In addition, a fundamental thermodynamic identity, such as

$$I = I(\rho, T) \quad (35)$$

is taken to reduce the number of unknowns to six (alternatively, we can view this as adding a seventh equation to the set). We have obtained six relations between the six unknown quantities, yielding a closed system.

See [7, 25, 30] for more detailed discussions of the thermodynamics of continuous media and state relations.

3.4 The Euler equations

In the case of an *ideal inviscid fluid*, there are by definition no shear or viscous stresses. In this case, $\bar{\mathbf{T}} = -p\bar{\mathbf{I}}$, and the momentum equations reduce to the *Euler equations*. Together with the equations for mass and energy, the system of governing equations becomes:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= \rho \mathbf{g} - \nabla p \\ \frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) &= -\nabla \cdot \mathbf{J} + \rho \mathbf{g} \cdot \mathbf{u} + q - \nabla \cdot (p \mathbf{u}).\end{aligned}$$

With the addition of the state equations, we have a closed system for the unknowns ρ , $\mathbf{u} = (u_1, u_2, u_3)$, p , and E .

3.5 The Navier-Stokes equations

In the case of *viscous fluids*, the viscous shear stress tensor $\bar{\sigma}$ is present, and the momentum equations are the full *Navier-Stokes equations*.

3.5.1 The compressible case

With the equations for mass and energy conservation, the full governing system is:

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= \rho \mathbf{g} - \nabla p + \nabla \cdot \bar{\sigma} \\ \frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) &= -\nabla \cdot \mathbf{J} + \rho \mathbf{g} \cdot \mathbf{u} + q - \nabla \cdot (p \mathbf{u}) + \nabla \cdot (\bar{\sigma} \cdot \mathbf{u}).\end{aligned}$$

A closed system results when the state equations are employed.

An analysis of the shear stresses in Newtonian fluids [7, 30] leads to the following form of the viscous shear stress tensor $\bar{\sigma}$:

$$\bar{\sigma} = 2\mu \operatorname{def} \mathbf{u} + \lambda \operatorname{div} \mathbf{u} \bar{\mathbf{I}} = \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \lambda(\nabla \cdot \mathbf{u})\bar{\mathbf{I}},$$

where μ and λ , the *first* and *second coefficients of viscosity*, respectively, depend on any two thermodynamic variables, for example the temperature and pressure. In particular, with this expression for the shear stress tensor $\bar{\sigma}$, the momentum equations can be written explicitly involving μ and λ as:

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{g} - \nabla p + \nabla(\lambda \nabla \cdot \mathbf{u}) + \nabla \cdot (\mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]).$$

3.5.2 The incompressible case

If μ and λ can be taken to be *constants*, then the momentum equations can be written as:

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \mathbf{g} - \nabla p + \nabla[(\lambda + \mu)\nabla \cdot \mathbf{u}] + \mu \nabla^2 \mathbf{u},$$

where we have used the equivalent non-conservation form involving the material derivative to express the left-hand side. If the fluid is *incompressible*, $\partial\rho/\partial t = 0$, and if the fluid has uniform density, expressed as $\nabla\rho = 0$, then the conservation of mass equation (28) or (31) clearly reduces to simply $\nabla \cdot \mathbf{u} = 0$. Using this result, the momentum equations become:

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \mathbf{g} - \nabla p + \mu \nabla^2 \mathbf{u}.$$

After dividing by the constant density ρ , and defining the *kinematic viscosity* $\nu = \mu/\rho$ and the *normalized pressure* $\bar{p} = p/\rho$, the *incompressible Navier-Stokes equations* result:

$$\frac{D\mathbf{u}}{Dt} = \frac{\partial\mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla\mathbf{u} = \mathbf{g} - \nabla\bar{p} + \nu\nabla^2\mathbf{u}.$$

Since ν and ρ are taken to be constants, coupling these equations with the conservation of mass equation $\nabla \cdot \mathbf{u} = 0$ gives four equations in the four unknowns \bar{p} and $\mathbf{u} = (u_1, u_2, u_3)$. In other words, the energy equation has been decoupled from the mass and momentum equations.

3.6 The governing equations of combustion

The equations governing combustion phenomena are based on the full compressible Navier-Stokes equations. In the case of a chemically reactive fluid consisting of N_c separate fluid species, the mass density ρ_m of each species m *changes* as chemical reactions take place. The total mass ρ will be the sum of the mass of individual chemical species, or $\sum_m \rho_m = \rho$. The governing equations of such a system must now incorporate mass conservation equations for each chemical species, in addition to the equation for the total mass.

3.6.1 Chemistry

As a chemical reaction takes place, one species may be converted into one or more others, giving rise to *mass source terms* $\dot{\rho}_m^c$ which were not otherwise present in the usual conservation of mass equation for a continuous medium. Energy or heat source terms \dot{Q}^c resulting from heat released during the kinetic chemical reactions also arise. These various source terms will appear in the equation for total energy as well as the equations for individual chemical species mass. Since mass is conserved in chemical reactions, an important constraint is that $\sum_m \dot{\rho}_m^c = 0$.

3.6.2 Sprays

We also consider one final complication: the possible injection of chemical species into the fluid, referred to as a *spray*. In addition to complications due to the chemistry, the governing equations must now also incorporate the effects of the spray, which will include an additional mass source term $\dot{\rho}_m^s$ for each injected species, a heat source term \dot{Q}^s due to spray interactions, and also a momentum source term \mathbf{F}^s induced by the spray. The total mass source due to the spray will be given by $\dot{\rho}^s = \sum_m \dot{\rho}_m^s$.

3.6.3 The modified source and flux terms

To employ the general conservation law forms of equations (9) and (10), we note that for the momentum equation, the above discussion yields a momentum volume source term of the form:

$$\mathbf{Q}_v = \rho\mathbf{g} + \mathbf{F}^s,$$

whereas the energy volume source term will have the form:

$$Q_v = \rho\mathbf{g} \cdot \mathbf{u} + q = \rho\mathbf{g} \cdot \mathbf{u} + (\dot{Q}^c + \dot{Q}^s).$$

The volume source term in the equation for conservation of total mass will take the form:

$$Q_v = \dot{\rho}^s,$$

and the volume source terms for individual species will be:

$$Q_v = \dot{\rho}_m^c + \dot{\rho}_m^s.$$

It can be shown [7] that the mass equations for individual species must now include a diffusive mass flux component of the form:

$$\mathbf{F}_d = -\rho D \nabla \left(\frac{\rho_m}{\rho} \right),$$

where the coefficient D is given by Fick's Law of diffusion.

3.6.4 The combustion equations

We will now write the governing equations using the general differential, conservation forms of equations (9) and (10); the various remaining source and flux terms will be exactly as in the Navier-Stokes equations discussed earlier. The resulting equations, representing conservation of mass, momentum, and energy, and reflecting the complications due to the chemistry and spray, are respectively:

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \cdot \left[\rho D \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s, \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{\rho}^s, \quad \sum_{m=1}^{N_c} \left(\frac{\rho_m}{\rho} \right) = 1$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{g} + \mathbf{F}^s - \nabla p + \nabla \cdot \bar{\sigma}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) = -\nabla \cdot \mathbf{J} + \rho \mathbf{g} \cdot \mathbf{u} + \dot{Q}^c + \dot{Q}^s - \nabla \cdot (p \mathbf{u}) + \nabla \cdot (\bar{\sigma} \cdot \mathbf{u}).$$

Alternatively, we can employ the internal energy equation in place of the equation for E :

$$\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\nabla \cdot \mathbf{J} + \dot{Q}^c + \dot{Q}^s - p \nabla \cdot \mathbf{u} + \bar{\sigma} : \nabla \mathbf{u}.$$

To obtain a closed system, we must employ the state relations as discussed earlier, and provide equations defining the source terms $\dot{\rho}_m^c$, $\dot{\rho}_m^s$, \mathbf{F}^s , \dot{Q}^c , and \dot{Q}^s . These will be discussed in more detail in the following sections.

More information on combustion theory in general may be found in [7, 14, 15].

3.7 Existence and uniqueness of solutions

Existence and uniqueness of solutions to the equations of fluid mechanics are important (and difficult) questions; see for example [31] for an analysis. A modern approach using a functional analysis setting for proving existence and uniqueness results in the case of the incompressible Navier-Stokes equations, as well as for analysis of numerical approximation methods, is given in [34].

4 The Governing Equations in KIVA-II

KIVA-II employs the combustion equations discussed in the previous section, with two additional features. First, the pressure gradient scaling (PGS) method [28] is used to improve computing efficiency for low Mach number flows (in which the pressure changes slowly), adding a scalar parameter of $1/\alpha^2$ to the pressure term in the momentum equations. Second, two turbulence modeling equations are coupled to the combustion equations via a scalar parameter A_0 .

If α is set to one, and A_0 is set to zero, then the combustion equations of the previous section are obtained. However, in KIVA-II, one constraint is that only a *single* chemical species, numbered $m = 1$, is injected into the fluid; hence, the term involving $\dot{\rho}_m^s$ in the individual mass conservation equations of the previous section has been changed to $\dot{\rho}_m^s \delta_{m1}$, where δ_{ij} is the Kronecker delta function.

4.1 The governing equations and unknowns

The following are the governing equations in KIVA-II for chemically reacting fluid flow in three-dimensions.

Conservation of mass:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{\rho}^s \quad (36)$$

Conservation of momentum (a vector equation with three components):

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = \rho \mathbf{g} + \mathbf{F}^s - \frac{1}{\alpha^2} \nabla p + \nabla \cdot \bar{\sigma} - A_0 \nabla \left(\frac{2}{3} \rho k \right) \quad (37)$$

Conservation of energy:

$$\frac{\partial(\rho I)}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = -\nabla \cdot \mathbf{J} + \dot{Q}^c + \dot{Q}^s - p \nabla \cdot \mathbf{u} + (1 - A_0) \bar{\sigma} : \nabla \mathbf{u} + A_0 \rho \epsilon \quad (38)$$

Turbulent kinetic energy:

$$\frac{\partial(\rho k)}{\partial t} + \nabla \cdot (\rho \mathbf{u} k) = -\frac{2}{3} \rho k \nabla \cdot \mathbf{u} + \bar{\sigma} : \nabla \mathbf{u} + \nabla \cdot \left[\left(\frac{\mu}{Pr_k} \right) \nabla k \right] - \rho \epsilon + \dot{W}^s \quad (39)$$

Turbulent kinetic energy dissipation:

$$\frac{\partial(\rho \epsilon)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \epsilon) = -\left(\frac{2}{3} c_{\epsilon_1} - c_{\epsilon_2} \right) \rho \epsilon \nabla \cdot \mathbf{u} + \nabla \cdot \left[\left(\frac{\mu}{Pr_\epsilon} \right) \nabla \epsilon \right] + \frac{\epsilon}{k} \left(c_{\epsilon_1} \bar{\sigma} : \nabla \mathbf{u} - c_{\epsilon_2} \rho \epsilon + c_s \dot{W}^s \right) \quad (40)$$

Heat flux:

$$\mathbf{J} = -K \nabla T - \rho D \sum_m h_m \nabla \left(\frac{\rho_m}{\rho} \right) \quad (41)$$

Equations of state:

$$p = R_0 T \sum_m \left(\frac{\rho_m}{\rho} \right) \quad (42)$$

$$I(T) = \sum_m \left(\frac{\rho_m}{\rho} \right) I_m(T) \quad (43)$$

$$c_p(T) = \sum_m \left(\frac{\rho_m}{\rho} \right) c_{pm}(T)$$

$$h_m(T) = I_m(T) + \frac{R_0 T}{W_m}$$

Mass consistency:

$$\sum_{m=1}^{N_c} \frac{\rho_m}{\rho} = 1 \quad (44)$$

Conservation of mass for chemical species m (one equation for each of the N_c species):

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}) = \nabla \cdot \left[\rho D \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s \delta_{m1} \quad (45)$$

The eleven equations (36) through (44), and N_c occurrences of equation (45) for N_c chemical species, yields $N_c + 11$ equations for the $N_c + 10$ unknowns ρ , $\mathbf{u} = (u_1, u_2, u_3)$, I , k , ϵ , \mathbf{J} , p , T , $\rho_1, \dots, \rho_{N_c}$. Since one of the mass equations is redundant due to the consistency equation, it is discarded, leaving $N_c + 10$ equations and unknowns.

The description of the unknowns is then:

$$\begin{aligned} \rho &= \sum_m \rho_m; \quad \text{total mass density} \\ \mathbf{u} &= (u_1, u_2, u_3); \quad \text{fluid velocity} \\ I &= \text{specific internal energy} \\ k &= \text{turbulent kinetic energy} \\ \epsilon &= \text{turbulent kinetic energy dissipation} \\ \mathbf{J} &= \text{heat flux vector} \\ p &= \text{fluid pressure} \\ T &= \text{temperature} \\ \rho_m &= \text{mass of chemical species } m = 1, \dots, N_c. \end{aligned}$$

4.1.1 Constants and parameters

The following is an explanation of all constants and parameters appearing in the governing equations. For a more detailed description of any particular parameter or constant, see [3].

$$\begin{aligned} h_m &= \text{enthalpy of chemical species } m = 1, \dots, N_c \\ c_p &= \text{specific heat at constant pressure} \\ V_m &= \rho_m / \rho; \quad \text{percent mass due to species } m \\ D &= \mu / (\rho S_c); \quad \text{diffusion coefficient from Fick's Law} \\ S_c &= \text{Schmidt number} \\ Pr &= \text{Prandtl number} \\ \mu &= (1.0 - A_0) \rho V_0 + \mu_{\text{air}} + A_0 c_\mu k^2 / \epsilon; \quad \text{first viscosity coefficient} \\ A_0 &= 0 \text{ for laminar model, } 1 \text{ for turbulence model} \\ \alpha &= \text{dimensionless quantity used with the PGS (pressure gradient scaling) method} \\ \mu_{\text{air}} &= A_1 T^{3/2} / (T + A_2); \quad \text{Sutherland formula for air viscosity} \\ c_\mu &= 0.09 \text{ (empirical constant)} \\ V_0 &= \text{input constant} \\ \lambda &= A_3 \mu; \quad \text{second viscosity coefficient} \\ A_3 &= -2/3 \text{ for turbulent flows, else arbitrary} \\ K &= \mu c_p / Pr; \quad \text{diffusion/transport coefficient} \\ W_m &= \text{molecular weight of species } m \\ I_m &= \text{specific internal energy of species } m \\ c_{pm} &= \text{specific heat at constant pressure of species } m \text{ (from JANAF tables)} \\ R_0 &= \text{universal gas constant} \\ \mathbf{g} &= \text{gravitational force} \\ \bar{\mathbf{I}} &= \text{unit tensor} \\ \delta_{m1} &= \text{Kronecker delta function, where species 1 is the spray droplet species} \\ \bar{\sigma} &= 2\mu \text{ def } \mathbf{u} + \lambda \text{ div } \mathbf{u} \bar{\mathbf{I}} = \mu [\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \lambda (\nabla \cdot \mathbf{u}) \bar{\mathbf{I}}; \quad \text{Viscous stress tensor.} \end{aligned}$$

4.1.2 Turbulence model constants

The following constants have been determined in various ways for turbulence modeling:

$$\begin{aligned}
c_{\epsilon_1} &= 1.44 \\
c_{\epsilon_2} &= 1.92 \\
c_{\epsilon_3} &= -1.0 \\
Pr_k &= 1.0 \\
Pr_\epsilon &= 1.3 \\
c_s &= 1.50.
\end{aligned}$$

Again, see [3] for a more detailed discussion of the turbulence model, and for a discussion of how these constants have been determined. We will not discuss the turbulence model any further in this report.

4.2 Source terms due to chemical reactions

The following source terms appear due to the chemical reactions.

$$\begin{aligned}
\dot{\rho}_m^c &= \text{mass density source term for species } m \text{ due to chemical reactions} \\
\dot{Q}^c &= \text{chemical heat release due to kinetic reactions.}
\end{aligned}$$

We now summarize the presentation in [3] regarding the forms and the calculation of the chemistry source terms, with additional material from [27] and [32].

The mass density source terms $\dot{\rho}_m^c$ depend on the reaction rates $\dot{\omega}_r$ for each reaction r in the following way:

$$\dot{\rho}_m^c = W_m \sum_r (b_{mr} - a_{mr}) \dot{\omega}_r$$

where reaction r is of the form:

$$\sum_m a_{mr} x_m \rightleftharpoons \sum_m b_{mr} x_m.$$

In this symbolic equation, x_m represents one mole of chemical species m , and a_{mr} and b_{mr} represent integer stoichiometric coefficients for species m in reaction r . For mass to be conserved, we must have for each reaction r that:

$$\sum_m (a_{mr} - b_{mr}) W_m = 0,$$

where W_m is the molecular weight of species m .

4.2.1 Equilibrium reactions

For *equilibrium reactions*, the reaction rates $\dot{\omega}_r$ are determined implicitly by the constraint that the mass densities ρ_m of all the chemical species satisfy the following relationship at all times:

$$\prod_m \left(\frac{\rho_m}{W_m} \right)^{b_{mr} - a_{mr}} = K_c^r(T),$$

where the *concentration equilibrium constant* K_c^r for reaction r takes the form:

$$K_c^r = e^{[A_r \ln T_A + (B_r/T_A) + C_r + D_r T_A + E_r T_A^2]},$$

for given constants A_r, B_r, C_r, D_r , and E_r . The parameter T_A is defined as a dimensionless scaling of the temperature, $T_A = T/1000K$.

4.2.2 Kinetic reactions

For *kinetic reactions*, the reaction rate $\dot{\omega}_r$ for reaction r is defined as:

$$\dot{\omega}_r = k_{fr} \prod_m \left(\frac{\rho_m}{W_m} \right)^{a'_{mr}} - k_{br} \prod_m \left(\frac{\rho_m}{W_m} \right)^{b'_{mr}},$$

where the coefficients involved are *Arrhenius* [3] in form:

$$k_{fr} = A_{fr} T^{\xi_{fr}} e^{-E_{fr}/T}$$

$$k_{br} = A_{br} T^{\xi_{br}} e^{-E_{br}/T}.$$

The constants A_{fr} , A_{br} , $T^{\xi_{fr}}$, and $T^{\xi_{br}}$ are defined for each reaction r and assumed given. The values E_{fr} and E_{br} are “activation temperatures” for reaction r . The stoichiometric coefficients a'_{mr} and b'_{mr} are allowed to vary from a_{mr} and b_{mr} to allow for the use of empirically determined reaction coefficients.

4.2.3 Chemical heat source terms

In the case of kinetic reactions, *chemical heat* is released. This heat is modeled with the heat source term \dot{Q}^c , which is introduced into the energy equation. The relationship between \dot{Q}^c and the reaction rates $\dot{\omega}_r$ is:

$$\dot{Q}^c = \sum_r Q_r \dot{\omega}_r.$$

In this expression, Q_r is the *negative* of the heat of reaction at absolute zero for reaction r :

$$Q_r = \sum_m (a_{mr} - b_{mr})(\Delta h_f^o)_m,$$

where the given parameter (Δh_f^o) is the *heat of formation* of species m at $T = 0$.

A discussion of the numerical procedures employed to compute the source terms due to chemical reactions at each time step in KIVA-II, using the above relationships, can be found in Appendix I (kinetic reactions) and Appendix J (equilibrium reactions) of [3].

4.3 Source terms due to the spray

The following source terms appear due to the spray.

$$\begin{aligned} \dot{\rho}_m^s &= \text{mass density source term due to sprayed species } m \\ \mathbf{F}^s &= \text{rate momentum gain per unit volume due to the spray} \\ \dot{Q}^s &= \text{heat source due to spray interactions} \\ \dot{W}^s &= \text{negative rate at which turbulent eddies do work dispersing spray droplets.} \end{aligned}$$

The three source terms, $\dot{\rho}_m^s$, \mathbf{F}^s , and \dot{Q}^s , represent an exchange of mass, momentum, and energy, respectively, between injected species $m = 1$ and the fluid. The fourth term listed above, \dot{W}^s , representing the dispersion of the spray droplets due to turbulent eddies, enters only into the turbulence modeling equations, and will not be discussed here. See [3] for a more detailed discussion of \dot{W}^s and the turbulence model.

4.3.1 The spray equation

For calculation of the remaining three source terms, KIVA-II employs the *spray equation formulation* [37], which is capable of representing drop collisions, oscillations, and dispersion. In the spray equation formulation, the spray droplets are represented by a *droplet probability distribution* $f(\mathbf{x}, \mathbf{v}, r, T_d, y, \dot{y})$. Here, \mathbf{x} and \mathbf{v} represent droplet position and velocity, r is the radius of a spherical droplet, T_d is the droplet temperature, y represents the amount of distortion from a sphere, and \dot{y} represents the distortion rate of change.

The droplet probability distribution function evolves according to the equation:

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot (f\mathbf{v}) + \nabla_{\mathbf{v}} \cdot (f\mathbf{F}) + \frac{\partial(fR)}{\partial r} + \frac{\partial(f\dot{T}_d)}{\partial T_d} + \frac{\partial(f\dot{y})}{\partial y} + \frac{\partial(f\ddot{y})}{\partial \dot{y}} = \dot{f}_{\text{coll}} + \dot{f}_{\text{bu}},$$

where the quantities \mathbf{F} , R , \dot{T}_d , and \dot{y} are rates of change of velocity, radius, temperature, and oscillation of an individual drop, respectively, and where \dot{f}_{coll} and \dot{f}_{bu} represent probability source terms due to droplet dispersion and collisions. The various expressions for these terms are given [3], along with a description of the numerical integration techniques employed.

4.3.2 Computing the spray source terms

Once f has been determined, the source terms due to the spray are given by approximating the following integrals:

$$\begin{aligned}\dot{\rho}^s &= - \int f \rho_d 4\pi r^2 R d\mathbf{v} dT_d dy dj, \\ \dot{\mathbf{F}}^s &= - \int f \rho_d \left(\frac{4}{3} \pi r^3 (\mathbf{F} - \mathbf{g}) + 4\pi r^2 R \mathbf{v} \right) d\mathbf{v} dr dT_d dy dj, \\ \dot{Q}^s &= - \int f \rho_d \left\{ 4\pi r^2 R [I_l(T_d)] + \frac{1}{2} (\mathbf{v} - \mathbf{u})^2 \right. \\ &\quad \left. + \frac{4}{3} \pi r^3 [c_l \dot{T}_d + (\mathbf{F} - \mathbf{g}) \cdot (\mathbf{v} - \mathbf{u} - \mathbf{u}')] \right\} d\mathbf{v} dr dT_d dy dj,\end{aligned}$$

where c_l and I_l are liquid specific heat and liquid internal energy, \mathbf{u}' is the gas turbulence velocity, and ρ_d is the liquid microscopic density.

A more detailed discussion of the parameters and constants appearing above, and a more detailed description of the spray droplet model in general, is given in [3].

4.4 Boundary conditions

Several types of boundary conditions are used in the KIVA-II implementation, and can be separated into physical and numerical conditions.

The allowed physical boundary conditions include inflow and outflow boundaries, periodic boundaries, and various wall boundary conditions. The wall boundary conditions include the possibility of a *wall velocity*, allowing for moving boundaries imposed by, for example, a moving piston in an internal combustion engine.

Numerical boundary conditions are often used in computational fluid mechanics for practical implementation reasons and are not a part of the original problem statement. These types of conditions are also used in KIVA-II to provide boundary conditions in several situations.

5 Discretization of the KIVA-II Equations

The discretization of the governing equations of combustion in KIVA-II involves a combination of the ALE or *Arbitrary Lagrangian-Eulerian* method for spatial discretization, and variably implicit time-discretization methods (or variable *theta-methods*).

5.1 Spatial discretization with the ALE method

The spatial discretization employed in KIVA-II is based on the ALE method [21]. This is a finite volume (FV) method, for arbitrary hexahedrons (or arbitrary four-sided polygons in two-dimensions). The equations of motion are formulated with a moving velocity \mathbf{U} , which varies from 0 to \mathbf{u} , yielding a continuous range of formulations from completely Eulerian ($\mathbf{U} = 0$) to completely Lagrangian ($\mathbf{U} = \mathbf{u}$).

The equations of motion developed in the previous sections, in differential, conservation form, are (ignoring chemistry, sprays, and viscosity for now):

$$\begin{aligned}\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \\ \frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \rho \mathbf{g} \\ \frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho \mathbf{u} E) &= -\nabla \cdot (p \mathbf{u}) + \rho \mathbf{g} \cdot \mathbf{u}.\end{aligned}$$

In integral form, with the ALE parameter \mathbf{U} , the equations become:

$$\begin{aligned}\frac{d}{dt} \int_{\Omega} \rho \, d\mathbf{x} - \oint_{\partial\Omega} \rho(\mathbf{U} - \mathbf{u}) \cdot \mathbf{n} \, ds &= 0 \\ \frac{d}{dt} \int_{\Omega} \rho \mathbf{u} \, d\mathbf{x} - \oint_{\partial\Omega} \rho \mathbf{u}(\mathbf{U} - \mathbf{u}) \cdot \mathbf{n} \, ds + \int_{\Omega} \nabla p \, d\mathbf{x} + \int_{\Omega} \rho \mathbf{g} \, d\mathbf{x} &= 0 \\ \frac{d}{dt} \int_{\Omega} \rho E \, d\mathbf{x} - \oint_{\partial\Omega} \rho E(\mathbf{U} - \mathbf{u}) \cdot \mathbf{n} \, ds + \oint_{\partial\Omega} p \mathbf{u} \cdot \mathbf{n} \, ds + \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{u} \, d\mathbf{x} &= 0.\end{aligned}$$

It is the integral forms that are discretized in the ALE method, as in the usual FV method.

What has changed is the introduction of the parameter \mathbf{U} into the governing equations. The equations are discretized in the standard way with the FV method, replacing the volume integrals with quadrature formulas, and enforcing continuity conditions across cell boundaries (which we define shortly) to cancel some of the surface integrals.

5.1.1 The ALE mesh and mesh parameters

We will discuss the ALE mesh in the two-dimensional case first; the extension to three dimensions follows easily. The two-dimensional ALE mesh is depicted in Figure 1.

In the ALE mesh, a *normal cell* is defined as the polygon in Figure (1) with the four vertices (i, j) , $(i + 1, j)$, $(i, j + 1)$, $(i + 1, j + 1)$, the mesh points at which are denoted $x_{i,j}$, $x_{i+1,j}$, $x_{i,j+1}$, $x_{i+1,j+1}$. The *cell center* is computed as

$$x_{ij}^c = \frac{1}{4} \sum_{\alpha} x_{\alpha}, \quad y_{ij}^c = \frac{1}{4} \sum_{\alpha} y_{\alpha},$$

where α ranges over the four cell vertices. Auxiliary cells, called *momentum cells*, are defined as surrounding a vertex x_{ij} , with cell edges meeting the midpoint of the surrounding regular cell edges, and vertices placed appropriately within the surrounding normal cells to cover one quarter each of the surrounding normal cell areas. There are then four faces or edges for each normal cell, and eight in the case of a momentum cell.

Normally, quantities assigned to vertices or mesh points x_{ij} are: $x, y, \mathbf{u} = (u_1, u_2)$, and the area of the momentum cell surrounding x_{ij} . Quantities assigned to cell centers x_{ij}^c are: cell areas V , pressure p , internal energy I , mass density ρ (or a cell mass $M = \rho V$). The three-dimensional case is the natural extension

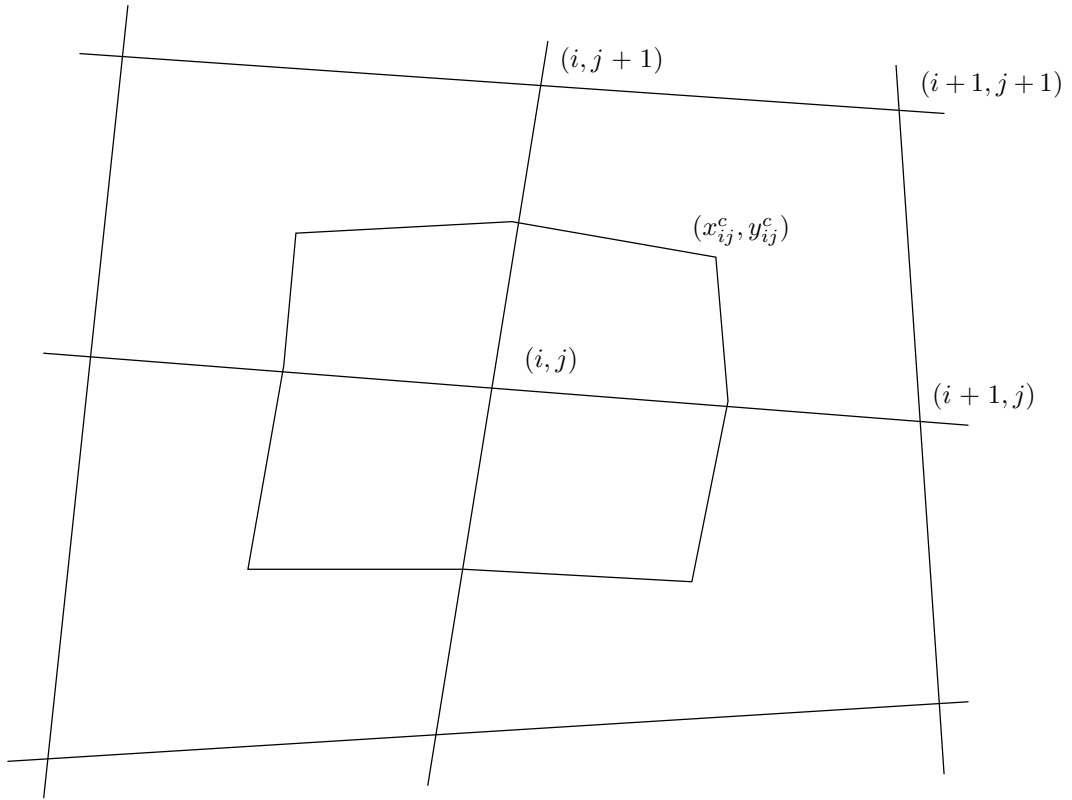


Figure 1: The two-dimensional ALE mesh.

of the two-dimensional version, and is outlined in [3]. The mesh vertices will be denoted now as x_{ijk} , and an additional velocity component for the third dimension, u_3 , will be defined at vertices. *Areas* in the above discussion will now refer to *volumes*, and *cell edges* will now become *cell faces*.

In the version of the ALE method implemented in KIVA-II, the velocities are also computed at the cell face centers of the normal cells. This is done to avoid parasitic modes in the velocity field that must otherwise be handled with a “node-coupling” technique [13].

In the finite volume discretization, several quantities having to do with the mesh must be computed. If the mesh moves in a Lagrangian fashion, then these quantities must be recomputed each time the mesh moves. The main quantities involved here are:

V_{ijk}	=	volume of normal cell (i, j, k) , computed from vertex positions
V'_{ijk}	=	volume of momentum cell (i, j, k)
M_{ijk}	=	mass of normal cell (i, j, k) , $M_{ijk} = \rho_{ijk} V_{ijk}$
M'_{ijk}	=	mass of momentum cell (i, j, k) , $M'_{ijk} = \rho_{ijk} V'_{ijk}$.
A_α	=	outward area vector associated with faces α for a normal cell (i, j, k)
A'_α	=	outward area vector associated with faces α for a momentum cell (i, j, k)
$(uA)_\alpha$	=	$\mathbf{u}_\alpha \cdot A_\alpha$; regular cell face normal velocities
$(uA')_\alpha$	=	$\mathbf{u}_\alpha \cdot A'_\alpha$; momentum cell face normal velocities.

In our presentation of the discrete equations to follow, values of an arbitrary function Q at a mesh point (i, j, k) will be denoted with the subscripts Q_{ijk} . If the function Q is to be evaluated at the center of a face rather than a normal mesh point, we denote it with a subscript α or β , such as Q_α .

5.1.2 The finite volume method

The spatial discretization is the standard FV discretization, performed by converting volume integrals to surface integrals (where possible) with the divergence theorem. Once this is done, the integrals are approximated with quadrature rules (i.e., function value at cell center times the cell volume to approximate the volume integral). Surface integrals over a cell become sums of integrals over cell faces (which again are approximated with quadrature; function value at face center times face area). In two-dimensions, we have of course surface and line integrals in place of volume and surface integrals, respectively.

Discretization error estimates for the finite volume method can be obtained in a rigorous fashion through difference and quadrature error formulas, as in [36] for the one and two dimensional cases.

As we are chiefly interested in those equations involved in the Phase B implicit solution, we will present only those discrete equations in detail. This will be done in §6, after a discussion of the temporal discretization. However, we will give one example here to illustrate the basic discretization, and to introduce the notation used later.

5.1.3 Example: the momentum equations

Consider equation (37), the momentum equations, written in the non-conservation form:

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \mathbf{g} + \mathbf{F}^s - \frac{1}{\alpha^2} \nabla p + \nabla \cdot \bar{\sigma} - A_0 \nabla \left(\frac{2}{3} \rho k \right).$$

For a (possibly moving) momentum cell $D(t) \subset \Omega$, the Lagrangian form of the equations is, in integral form:

$$\frac{d}{dt} \int_{D(t)} \rho \mathbf{u} \, d\mathbf{x} = \int_{D(t)} \rho \mathbf{g} \, d\mathbf{x} + \int_{D(t)} \mathbf{F}^s \, d\mathbf{x} - \frac{1}{\alpha^2} \oint_{\partial D(t)} p \mathbf{n} \, ds + \oint_{\partial D(t)} \mathbf{n} \cdot \bar{\sigma} \, ds - A_0 \frac{2}{3} \oint_{\partial D(t)} \rho k \mathbf{n} \, ds,$$

where we have converted some of the volume integrals to surface integrals with the divergence theorem. We now approximate the remaining volume integrals with the function evaluated at the mesh point x_{ijk} times the volume of the momentum cell D . The surface integrals are approximated with the sums of the area integrals over the faces of the momentum cell, each of which is approximated with the function value at a face center times the face area.

If we denote the sum of the area integrals as \sum_{β} , where β ranges over the cell faces, then the above equation is semi-discretized in space as:

$$\frac{d}{dt} [(\rho_{ijk} \mathbf{u}_{ijk}) V'_{ijk}] = \rho_{ijk} \mathbf{g}_{ijk} V'_{ijk} + \mathbf{F}^s_{ijk} V'_{ijk} - \frac{1}{\alpha^2} \sum_{\beta} p_{\beta} (A')_{\beta} + \sum_{\beta} \bar{\sigma}_{\beta} \cdot (A')_{\beta} - A_0 \frac{2}{3} \sum_{\beta} \rho_{\beta} k_{\beta} (A')_{\beta}.$$

Defining the *momentum cell mass* $M'_{ijk} = \rho_{ijk} V'_{ijk}$, we obtain:

$$\frac{d}{dt} [(M')_{ijk} \mathbf{u}_{ijk}] = \mathbf{g}_{ijk} (M')_{ijk} + \mathbf{F}^s_{ijk} V'_{ijk} - \frac{1}{\alpha^2} \sum_{\beta} p_{\beta} (A')_{\beta} + \sum_{\beta} \bar{\sigma}_{\beta} \cdot (A')_{\beta} - A_0 \frac{2}{3} \sum_{\beta} \rho_{\beta} k_{\beta} (A')_{\beta}.$$

Note that the time derivative will introduce the usual advection term via the transport theorem.

The remaining equations (36) through (44), and N_c occurrences of equation (45), are semi-discretized in space in a similar fashion.

5.2 Temporal discretization with variably implicit schemes

In KIVA-II, all time derivatives are approximated with the first-order difference:

$$\frac{\partial Q}{\partial t} \approx \frac{Q^{n+1} - Q^n}{\Delta t^n},$$

where $Q(t)$ is some function evolving in the simulation, $Q^n = Q(t^n)$, and $\Delta t^n = t^{n+1} - t^n$. Each time step is performed in three phases; the results of the first phase, given superscript A, for example Q^A , are used in the second phase, which in turn produces results Q^B , and so forth. The flow of the computation is then:

$$Q^n \longrightarrow Q^A \longrightarrow Q^B \longrightarrow Q^{n+1}.$$

Intermediate values, updated for example by an equation of state at some point in the time-stepping, are denoted as Q^t or as \tilde{Q} .

5.2.1 Theta-methods

Time discretization of the governing equations in KIVA-II is performed in a *variably implicit fashion*, employing *implicitness parameters*. These parameters allow the discretization to produce a continuous range of approximations, from fully explicit to fully implicit.

In the KIVA-II documentation, the implicitness parameters are denoted as Φ , with a subscript indicating the quantity involved; for example, Φ_p will refer to a term involving the pressure p . This class of methods is sometimes referred to as the *theta-methods* [1] in the literature, where Θ is used to represent the implicitness parameter. For example, the Crank-Nicolson method is a theta-method with $\Theta = \frac{1}{2}$, whereas $\Theta = 1$ yields the backward Euler method. A generalization of a standard theta-method employed in KIVA-II allows for Θ to vary with time.

Below, we explain how the time discretization is performed, using again the momentum equations as an example. In §6, we will present in detail the forms of the fully discretized equations involved in the Phase B implicit solution procedure.

5.2.2 Example: the momentum equations

As an example of the variably implicit time-stepping schemes employed, consider again the momentum equations, which when semi-discretized in space as in the previous section, take the form:

$$\frac{d}{dt}[(M')_{ijk} \mathbf{u}_{ijk}] = \mathbf{g}_{ijk}(M')_{ijk} + \mathbf{F}_{ijk}^s V'_{ijk} - \frac{1}{\alpha^2} \sum_{\beta} p_{\beta}(A')_{\beta} + \sum_{\beta} \bar{\sigma}_{\beta} \cdot (A')_{\beta} - A_0 \frac{2}{3} \sum_{\beta} \rho_{\beta} k_{\beta}(A')_{\beta}.$$

If we now employ a theta-method for time discretization, we obtain the fully discretized equation:

$$\begin{aligned} \frac{(M')_{ijk}^{n+1} \mathbf{u}_{ijk}^{n+1} - (M')_{ijk}^n \mathbf{u}_{ijk}^n}{\Delta t} &= \mathbf{g}_{ijk}(M')_{ijk}^n + (\mathbf{F}_{ijk}^s V'_{ijk})^n - \frac{1}{(\alpha^n)^2} \sum_{\beta} [\Phi_p p^{n+1} + (1 - \Phi_p) p^n]_{\beta} (A')_{\beta}^n \\ &+ \sum_{\beta} [\Phi_D \bar{\sigma}(\mathbf{u}^{n+1}) + (1 - \Phi_D) \bar{\sigma}(\mathbf{u}^n)]_{\beta} \cdot (A')_{\beta}^n - A_0 \frac{2}{3} \sum_{\beta} \rho_{\beta}^n k_{\beta}^n (A')_{\beta}^n. \end{aligned}$$

The parameters Φ_p and Φ_D are the implicitness parameters, set to zero for a fully explicit method, and to one for a fully implicit method. Finally, note that the transport theorem requires the introduction of an advection term (which is nonlinear) on the left-hand side of the above equation. In KIVA-II, this advection term is computed in a fully explicit fashion in a separate phase of the computation.

The remaining equations (36) through (44), and N_c occurrences of equation (45), are discretized in time in a similar, variably implicit, fashion.

5.3 The overall time-stepping structure

Each time-step is broken into three separate *phases*: Phase A, consisting mainly of chemistry and droplet interactions; Phase B, consisting of fluid diffusion and droplet velocity calculations; and Phase C, in which the fluid is advected and the mesh is rezoned. In addition, there is some initialization before the first time-step, and before each time step thereafter. The most time-consuming phase is the implicit fluid diffusion calculated in Phase B, which we will discuss in more detail later on. The overall structure is depicted in Figure 2.

5.3.1 Initialization

At the outset of the simulation, KIVA-II performs the following initialization steps:

1. initialize all variables

2. compute all required parameters
3. read user input and problem specification
4. create the mesh and cell variables.

In addition, at the beginning of each subsequent time step, KIVA-II performs the additional initialization:

1. calculate viscosity
2. calculate all area projections
3. determine the appropriate time step
4. reinitialize cell variables.

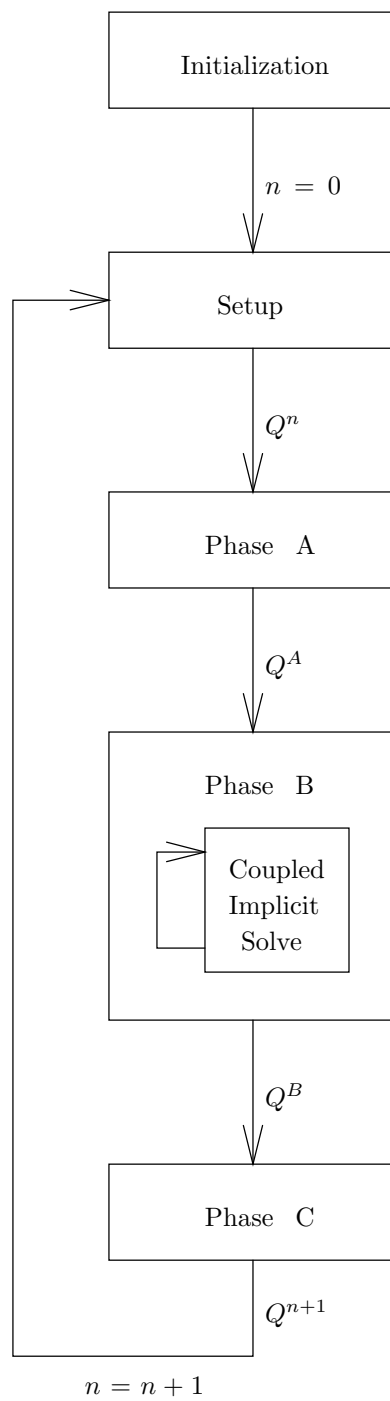


Figure 2: The basic KIVA-II time-stepping structure.

5.3.2 Phase A – chemistry and spray droplet interactions

Phase A consists mainly of calculating the effects of chemical reactions and spray droplet interactions due to species 1 being injected into the fluid. The overall structure of this phase is as follows:

- spray effects
 1. droplet injection
 2. move the piston (engine simulations only)
 3. calculation of spray droplet transport and turbulence
 4. calculation of spray droplet breakup
 5. compute droplet collisions
 6. determine drop evaporation
- chemistry effects
 1. chemical kinetic and ignition reactions
 2. equilibrium reactions
- additional spray effects
 1. gravity effects
 2. droplet mass, momentum, and energy couplings.

5.3.3 Phase B – fluid diffusion and droplet velocity calculations

Phase B consists mainly of fluid calculations, with some additional spray effects due to the momentum coupling of the droplets to the fluid. Fluid diffusion is calculated in this phase implicitly, while fluid advection is calculated explicitly in Phase C. The flow of computation in Phase B is:

- preliminary fluid effects
 1. mass diffusion
 2. viscous stress calculation
 3. predicted (extrapolated) pressure
- primary fluid calculation – a coupled implicit solve which is performed iteratively
 1. implicit momentum diffusion
 2. implicit heat diffusion
 3. pressure solution
- additional fluid effects
 1. calculate densities, energy, and Lagrangian coordinates
 2. implicit diffusion of turbulent energy and dissipation
- update of droplet velocities.

5.3.4 Phase C – fluid advection and mesh rezoning

The fluid advection calculation is performed Phase C, while the remainder of the phase is primarily book-keeping and preparing for the next time step. The structure of the computation is:

- grid updating
 1. calculation of grid velocities
 2. rezoning of the grid
 3. new cell volumes and area projections
- fluid advection
 1. explicit advection of mass, energy, and turbulent energy
 2. explicit advection of momentum
- additional grid details
- equations of state.

Note that in the version of ALE implemented in KIVA-II, the rezoning calculation in Phase C is always performed, although it is optional in the usual ALE method.

6 The Coupled Implicit Phase B Solution in KIVA-II

To obtain “time-advanced” pressure forces in the Lagrangian part of the calculation, an implicit diffusion iteration is performed, referred to as *an outer iteration*. In an explicit method, pressure forces can only advance one cell at each time step. If the time step is chosen large enough that sound waves should travel *more* than a single cell, then inaccuracy and instability results. See [21] for a more complete discussion of this problem.

6.1 The SIMPLE algorithm

In an ideal situation, velocities at a new time step in a numerical simulation would be computed from time-advanced pressure gradients. To use *time-advanced* pressures requires an iterative solution procedure, because the pressures depend on accelerations and velocities computed from the pressures. The original algorithm incorporating time advanced pressures, referred to as the SIMPLE [3, 32] algorithm, was as follows:

1. compute V^* , the volume of cell (i, j, k) , after moving the cell with current velocity \mathbf{u}
2. compute approximations for ρ and I using V, V^*, p, I, ρ
3. compute a pressure correction p^c using ρ, I, p
4. compute new velocities \mathbf{u} from p^c
5. if $(\|p - p^c\| < \text{TOL})$ quit; else goto 1.

The modified version of this coupled implicit solution algorithm employed in KIVA-II is depicted in Figure 3. This version involves extrapolation of the pressure, followed by iterative solution of equations for the velocities, the temperature, and finally the pressure.

In the following, we will give the full discrete equations for various parts of the Phase B computations. Most of the terms and notations have been previously explained earlier in the report. A few previously undefined terms will appear, which we will explain as necessary.

6.2 Predicted pressure by extrapolation

The predicted pressure is computed in the PINIT subroutine, according to the extrapolation formula (see equation 108, page 45 of [3]):

$$p_{ijk}^p = (p_{ijk}^B)^{n-1} + \frac{\Delta t^n}{\Delta t^{n-1}} [(p_{ijk}^B)^{n-1} - (p_{ijk}^B)^{n-2}].$$

Note that $(p^B)^{n-1}$ is the Phase B pressure from the previous time step $n - 1$.

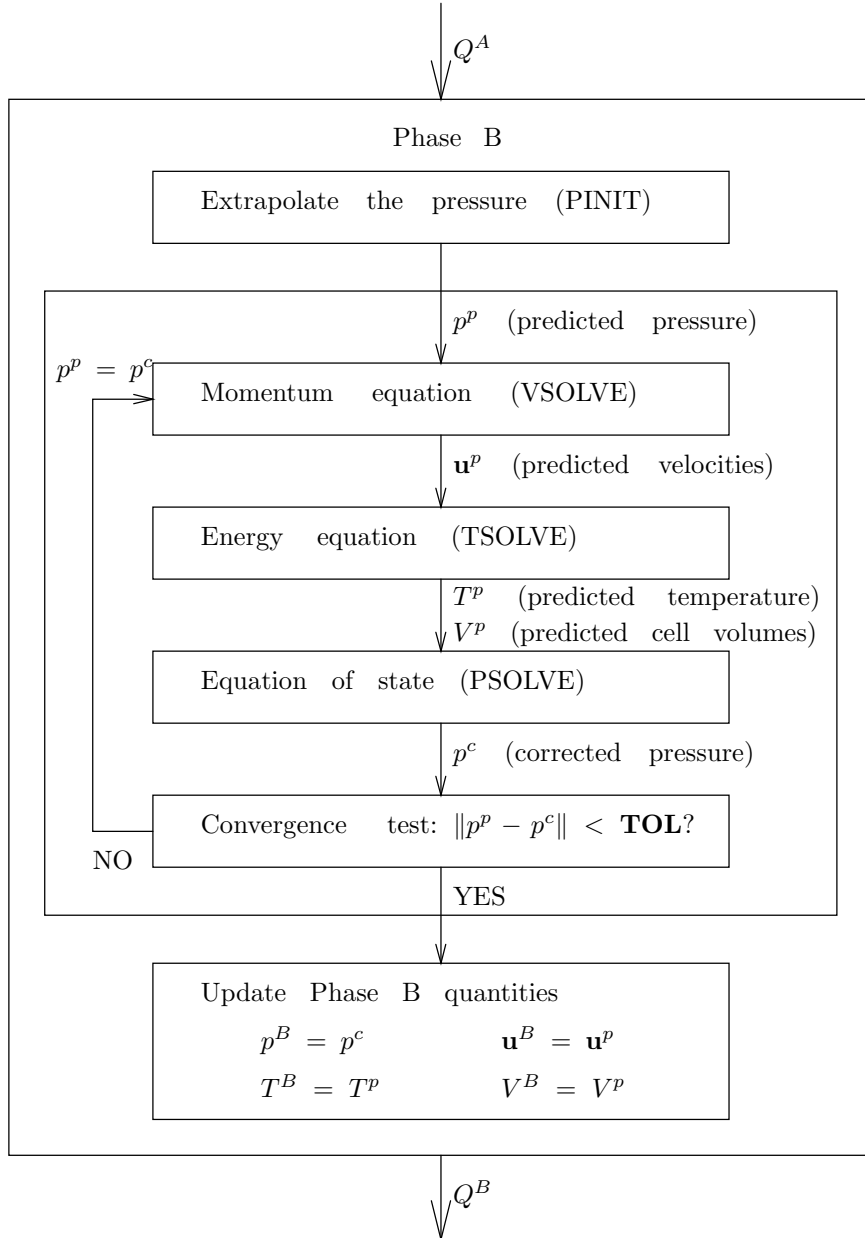


Figure 3: The Phase B coupled implicit solve in KIVA-II.

6.3 Predicted velocities from the momentum equations

The predicted velocities are computed in the VSOLVE subroutine, by solving the momentum equations after employing the previously predicted pressures (see equation 78, page 36 of [3]):

$$\begin{aligned} \frac{(M')_{ijk}^B \mathbf{u}_{ijk}^p - (M')_{ijk}^n \mathbf{u}_{ijk}^n}{\Delta t} = & -\frac{1}{(\alpha^n)^2} \sum_{\beta} [\Phi_p p^p + (1 - \Phi_p) p^n]_{\beta} (A')_{\beta}^n - A_0 \sum_{\beta} \frac{2}{3} \rho_{\beta}^A \kappa_{\beta}^A (A')_{\beta}^n \\ & + \sum_{\beta} [\Phi_D \bar{\sigma}(\mathbf{u}^p) + (1 - \Phi_D) \bar{\sigma}(\mathbf{u}^n)]_{\beta} \cdot (A')_{\beta}^n \\ & - \frac{1}{\Delta t} (R'_{ijk} + S'_{ijk} \mathbf{u}_{ijk}^p) + \mathbf{g} (M')_{ijk}^n - (M')_{ijk}^n (ANC)_{ijk} / \Delta t. \end{aligned}$$

The quantity ANC represents the *alternate node coupler* used to control parasitic pressure modes, which is described in Appendix L of [3]. The parameter Φ_p is an *implicitness* parameter which allows the discretization to vary between fully explicit and fully implicit. A procedure for computing Φ_p automatically from stability considerations is outline in Appendix H of [3].

The only quantities in the above that remain to be defined are R'_{ijk} and S'_{ijk} , which arise in the coupling of the gas and droplet velocities through the momentum source term \mathbf{F}^s of equation (37). Expressions for each are given in Appendix C of [3].

The above equation is linear in \mathbf{u}_{ijk}^p , and of the form:

$$\sum_{\beta} [\Phi_D \bar{\sigma}(\mathbf{u}^p)] \cdot (A')_{\beta}^n + [(M')_{ijk}^B + S'_{ijk}] \mathbf{u}_{ijk}^p = \mathbf{F}_{\mathbf{u}}(\mathbf{u}_{ijk}^n, p^p, p^n, \dots).$$

In KIVA-II, this linear system is solved with the conjugate residual method, which we will describe shortly.

6.4 Predicted temperature from the energy equation

The predicted temperature is computed in the TSOLVE subroutine, by solving the following equation which is obtained by combining the energy equation with an equation of state and the momentum equations (see equation 110, page 46 of [3]):

$$\begin{aligned} T_{ijk}^p = & \left\{ T_{ijk}^t + \frac{p_{ijk}^n + p_{ijk}^p}{2(c_v)_{ijk}^t} \cdot \frac{V_{ijk}^n}{M_{ijk}^B} + \frac{\Delta t}{M_{ijk}^B (c_v)_{ijk}^t} \left[\sum_{\alpha} K_{\alpha}^n \nabla [\Phi_D T^p + (1 - \Phi_D) \tilde{T}]_{\alpha} \cdot A_{\alpha}^n \right. \right. \\ & \left. \left. + (1 - A_0) [\Phi_D \bar{\sigma}(\mathbf{u}^p) : \nabla \mathbf{u}^p + (1 - \Phi_D) \bar{\sigma}(\mathbf{u}^n) : \nabla \mathbf{u}^n]_{ijk} \right] \right\} \\ & / \left\{ 1 + \frac{p_{ijk}^n + p_{ijk}^p}{2(c_v)_{ijk}^t p_{ijk}^p} R_0 \left[\sum_m \frac{(Y_m)_{ijk}^B}{W_m} \right] \right\}. \end{aligned}$$

The terms T^t and \tilde{T} are updated values from the equations of state. The parameter Φ_D is again a variable implicitness parameter, computed dynamically.

The above equation, linear in T_{ijk}^p , can be written in the form:

$$\frac{\Delta t}{M_{ijk}^B (c_v)_{ijk}^t} \left[\sum_{\alpha} K_{\alpha}^n \nabla [\Phi_D T^p] \cdot A_{\alpha}^n \right] + T_{ijk}^p = \mathbf{F}_T(p_{ijk}^n, p_{ijk}^p, \mathbf{u}^p, \mathbf{u}^n, \dots).$$

This equation is also solved with a conjugate residual method.

The subroutine TSOLVE also produces new predicted cell volumes using the predicted temperature, by employing the equation (see equation 111, page 46 of [3]):

$$V_{ijk}^p = \frac{M_{ijk}^B}{P_{ijk}^p} R_0 \left[\sum_m \frac{(Y_m)_{ijk}^B}{W_m} \right] T_{ijk}^p.$$

6.5 Corrected pressure

Calculation of the corrected pressure p_{ijk}^c involves the simultaneous solution of equations for:

1. corrected cell face velocities, uA^c
2. corrected cell volumes, V_{ijk}^c
3. corrected pressure, p_{ijk}^c .

6.5.1 Cell face velocity equation

The cell face velocity equation is (see equation 86, page 38 of [3]):

$$\begin{aligned} [(M'')_{\alpha}^B + S''] \frac{(uA)_{\alpha}^c - (uA)_{\alpha}^t}{\Delta t} = - \sum_{\beta} \left\{ [\Phi_p p^c + (1 - \Phi_p) p^n] / (\alpha^n)^2 + A_0 \frac{2}{3} \rho^A \kappa^A \right\}_{\beta} (A'')_{\beta}^n \cdot A_{\alpha} \\ + \frac{A_{\alpha}^t - A_{\alpha}^n}{\Delta t} \cdot \frac{\mathbf{u}_a^n + \mathbf{u}_b^n + \mathbf{u}_c^n + \mathbf{u}_d^n}{4} [(M'')_{\alpha}^B + S'']. \end{aligned}$$

The parameter Φ_p is a variable implicitness parameter. The velocities \mathbf{u}_x^n refer to the velocity \mathbf{u} at the four corners of the cell face identified by α . The double-primed variables refer to a cell face control volume rather than a regular or momentum cell; otherwise their meanings are as in the single- or un-primed case.

This is a linear equation in the unknowns $(uA)_{\alpha}^c$ and p_{ijk}^c , and can be written in the form:

$$[(M'')_{\alpha}^B + S''] (uA)_{\alpha}^c + \frac{\Delta t}{(\alpha^n)^2} \sum_{\beta} \Phi_p p^c = \mathbf{F}_1((uA)_{\alpha}^t, p^n, \rho^A, A_{\alpha}^t, A_{\alpha}^n, \mathbf{u}, \dots).$$

6.5.2 Cell volume equation

The following equation (equation 102, page 42 of [3]) is used to obtain corrected cell volumes from the corrected cell face velocities:

$$V_{ijk}^c = V_{ijk}^n + \Delta t \sum_{\alpha} (uA)_{\alpha}^c.$$

This equation is linear in the two unknowns V_{ijk}^c and $(uA)_{\alpha}^c$, and can be written in the form:

$$V_{ijk}^c - \Delta t \sum_{\alpha} (uA)_{\alpha}^c = \mathbf{F}_2(V_{ijk}^n).$$

6.5.3 A linearized equation of state

The third equation which couples with the two above is obtained after combining the original discretized equation of state for p with the temperature equation above, ignoring the diffusion terms in the temperature equation, and linearizing about the cell volumes and pressures (see equation 112, page 46 of [3]):

$$V_{ijk}^c = V_{ijk}^p - \frac{1}{\gamma_{ijk}^t} \cdot \frac{V_{ijk}^p}{p_{ijk}^p} (p_{ijk}^c - p_{ijk}^p),$$

where the term involving γ_{ijk}^t is given by:

$$\frac{1}{\gamma_{ijk}^t} = \frac{2(c_v)_{ijk}^t + R_0 \left[\sum_m \frac{(Y_m)_{ijk}^B}{W_m} \right] \left(1 - \frac{V_{ijk}^n}{V_{ijk}^p} \right)}{2(c_v)_{ijk}^t + \frac{p_{ijk}^n + p_{ijk}^p}{p_{ijk}^p} R_0 \left[\sum_m \frac{(Y_m)_{ijk}^B}{W_m} \right]}.$$

This equation is linear in V_{ijk}^c and p_{ijk}^c , and can be written as:

$$V_{ijk}^c + \left[\frac{1}{\gamma_{ijk}^t} \cdot \frac{V_{ijk}^p}{p_{ijk}^p} \right] p_{ijk}^c = \mathbf{F}_3(V_{ijk}^p, p_{ijk}^p, p_{ijk}^n, V_{ijk}^n, \dots).$$

The three equations above are solved in a coupled fashion with the conjugate residual method.

6.6 The conjugate residual method

We wish to solve the linear system $Ax = b$, given an initial approximation x_0 to x . A *conjugate gradient (CG) method* for solving this system, implemented using the *Omin algorithm* [8], has the form given in the left box of Figure 4. It is shown in [8] that any CG method may be characterized by the three matrices B , C , and A , where B is an Hermitian positive definite (hpd) inner product matrix, C is a preconditioning matrix, and A is the system matrix. In the Omin algorithm, the notation $\langle \cdot, \cdot \rangle$ represents the Euclidean inner product of two vectors. The quantity $e_i = x - x_i$ represents the (unknown) error in approximation x_i at step i , and the method is *computable* only if $\langle Be_i, p_i \rangle$ is computable. (The quantity Ae_{i+1} appearing is always computable since it is equal to the residual r_{i+1} .)

<u>The Omin Algorithm</u>	<u>The Omin Implementation of PCR</u>
Given x_0 ;	Given x_0 ;
Initialize: $r_0 = b - Ax_0$, $p_0 = Cr_0$	Initialize: $r_0 = b - Ax_0$, $p_0 = Cr_0$
Do $i = 0, 1, 2, \dots$ until convergence:	Do $i = 0, 1, 2, \dots$ until convergence:
$\alpha_i = \frac{\langle Be_i, p_i \rangle}{\langle Bp_i, p_i \rangle}$	$\alpha_i = \frac{\langle r_i, CAp_i \rangle}{\langle CAp_i, Ap_i \rangle}$
$x_{i+1} = x_i + \alpha_i p_i$	$x_{i+1} = x_i + \alpha_i p_i$
$r_{i+1} = r_i - \alpha_i Ap_i$	$r_{i+1} = r_i - \alpha_i Ap_i$
$s_{i+1} = Cr_{i+1}$	$s_{i+1} = Cr_{i+1}$
$\beta_i = -\frac{\langle BC Ae_{i+1}, p_i \rangle}{\langle Bp_i, p_i \rangle}$	$\beta_i = -\frac{\langle As_{i+1}, CAp_i \rangle}{\langle CAp_i, Ap_i \rangle}$
$p_{i+1} = s_{i+1} + \beta_i p_i$	$p_{i+1} = s_{i+1} + \beta_i p_i$

Figure 4: The Omin algorithm for a general CG method, and for PCR.

The special case referred to as the *preconditioned conjugate residual method* (preconditioned CR, or PCR) arises with the choice of the inner product matrix $B = ACA$, where C is some appropriate preconditioner. The Omin algorithm implementing this method is guaranteed to converge (in n steps, if A is $n \times n$) for hpd matrices A and C , and has the form given in the right box of Figure 4. The Hermitian properties of A and C have been used in some places to obtain alternate expressions, which are then either computable, or possibly more efficient by reusing previously computed quantities.

Note that if A is only Hermitian (not positive definite), then a more robust algorithm, referred to as *Odin* [8], must be employed to guarantee convergence of PCR; we discuss only the Omin algorithm here. Since we are concerned only with real (not complex) linear systems $Ax = b$ and preconditioners C , the conditions for convergence of the Omin implementation of PCR are that each of B , C , and A be symmetric positive definite (spd). See [8] for more information about CG methods.

While the Phase B portions of the KIVA-II software are organized somewhat differently than the original KIVA (including different subroutine names, additional subroutines, and differing logical structure), the algorithm implementing PCR in KIVA-II is essentially as described in [26] for the original KIVA. At first glance, this algorithm appears to be far different from the Omin implementation of PCR above; however, it is equivalent to the Omin algorithm. In the following discussion, we will use a different notation than that used in [26] to be consistent with the numerical analysis literature on CG methods.

First, note that in the Omin algorithm, the matrix A representing the linear system $Ax = b$ must be applied to the vectors p_i and s_i , the *direction* and *preconditioned residual vectors*, respectively. To apply A to s_i , note that:

$$As_i = A(s_i + x_i - x_i) + b - b = b - Ax_i + A(x_i + s_i) - b = r_i - [b - A(x_i + s_i)].$$

<u>Modified Omin/PCR Algorithm</u>	<u>KIVA-II Version of Omin/PCR</u>
Given x_0 ; Initialize: $r_0 = b - Ax_0$, $s_0 = Cr_0$ $p_0 = s_0$, $\bar{r}_0 = b - A(x_0 + s_0)$ $As_0 = r_0 - \bar{r}_0$, $Ap_0 = As_0$ Do $i = 0, 1, 2, \dots$ until convergence: $\alpha_i = \frac{\langle r_i, CAp_i \rangle}{\langle CAp_i, Ap_i \rangle}$ $x_{i+1} = x_i + \alpha_i p_i$ $r_{i+1} = r_i - \alpha_i Ap_i$ $s_{i+1} = Cr_{i+1}$ $\bar{r}_{i+1} = b - A(x_{i+1} + s_{i+1})$ $As_{i+1} = r_{i+1} - \bar{r}_{i+1}$ $\beta_i = -\frac{\langle As_{i+1}, CAp_i \rangle}{\langle CAp_i, Ap_i \rangle}$ $p_{i+1} = s_{i+1} + \beta_i p_i$ $Ap_{i+1} = As_{i+1} + \beta_i Ap_i.$	Given x_0 ; Initialize: $r_0 = b - Ax_0$, $\beta_{-1} = 0$ $p_{-1} = 0$, $Ap_{-1} = 0$ Do $i = 0, 1, 2, \dots$ until convergence: $s_i = Cr_i$ $\bar{r}_i = b - A(x_i + s_i)$ $As_i = r_i - \bar{r}_i$ $\beta_{i-1} = -\frac{\langle As_i, CAp_{i-1} \rangle}{\langle CAp_{i-1}, Ap_{i-1} \rangle} \quad (i > 0)$ $p_i = s_i + \beta_{i-1} p_{i-1}$ $Ap_i = As_i + \beta_{i-1} Ap_{i-1}$ $\alpha_i = \frac{\langle r_i, CAp_i \rangle}{\langle CAp_i, Ap_i \rangle}$ $x_{i+1} = x_i + \alpha_i p_i$ $r_{i+1} = r_i - \alpha_i Ap_i.$

Figure 5: A modified Omin algorithm for PCR, and as implemented in KIVA-II.

Once As_i is computed, Ap_i can be computed from the definition of p_i :

$$Ap_i = A(s_i - \beta_{i-1} p_{i-1}) = As_i - \beta_{i-1} Ap_{i-1}.$$

Since Ap_{i-1} is available from the previous iteration, this involves only vector subtraction. Therefore, if the residual of the system $Ax = b$ can be computed with the approximation $\bar{x}_i = x_i + s_i$, which we will denote as $\bar{r}_i = b - A\bar{x}_i = b - A(x_i + s_i)$, then As_i and Ap_i can be computed as $As_i = r_i - \bar{r}_i$, and $Ap_i = As_i - \beta_{i-1} Ap_{i-1}$.

In other words, the Omin implementation of PCR can be formulated with a single (modified) residual calculation at each iteration, rather the explicit application of the matrix A . The resulting modified algorithm has the form given in the left box of Figure 5. This formulation of PCR is useful if it is easier to form the residual of the linear system than it is to identify and apply the system matrix A . Such is the case in KIVA-II, especially for the coupled implicit solve for the corrected pressure.

The preconditioning matrix C has yet to be defined. To improve the convergence rate of a CG method, C is usually chosen to be some approximation to the inverse of A . In KIVA-II, it is taken to be the diagonal of the matrix A , referred to as *Jacobi preconditioning*, or simply as diagonal scaling. While it is difficult to identify the matrix A in the KIVA-II application, both the residual $r_i = b - Ax_i$ and the diagonal of A are computable.

In order to finally specify the form of the Omin algorithm used in KIVA-II to implement PCR, we note that the Omin algorithm in the left box of Figure 5 may be reordered slightly, leaving a mathematically equivalent algorithm. A simple rearrangement and change in the subscripts gives the algorithm in the right box of Figure 5; it is easily verified by inspection that the two algorithms produce the same sequence of iterates x_i . The Omin algorithm in the right box of Figure 5 is used for all of the implicit linear solves in the KIVA-II software.

Note that since A must be spd for convergence of the Omin implementation of PCR, and since the boundary conditions in the KIVA-II governing equations may create nonsymmetries in the resulting discretized linear operators, the method is not guaranteed to converge. However, in practice the iteration converges, and quite rapidly, for the two linear systems describing the temperature and velocities.

In the case of the corrected pressures, however, the situation is somewhat more complex. We are faced with three linear equations coupling the three unknowns p_{ijk}^c , V_{ijk}^c , and $(uA)_\alpha^c$, which are of the form:

$$[(M'')_\alpha^B + S''_\alpha](uA)_\alpha^c + \frac{\Delta t}{(\alpha^n)^2} \sum_\beta \Phi_p p^c = \mathbf{F}_1((uA)_\alpha^t, p^n, \rho^A, A_\alpha^t, A_\alpha^n, \mathbf{u}, \dots) \quad (46)$$

$$V_{ijk}^c - \Delta t \sum_\alpha (uA)_\alpha^c = \mathbf{F}_2(V_{ijk}^n) \quad (47)$$

$$V_{ijk}^c + \left[\frac{1}{\gamma_{ijk}^t} \cdot \frac{V_{ijk}^p}{p_{ijk}^p} \right] p_{ijk}^c = \mathbf{F}_3(V_{ijk}^p, p_{ijk}^p, p_{ijk}^n, V_{ijk}^n, \dots). \quad (48)$$

The following is an outline of how PCR is formulated for the corrected pressures p^c , based on the modified Omin algorithm in the right box of Figure 5.

The PCR method for the corrected pressures is performed as a single loop in the **PSOLVE** subroutine. At iteration v , the subroutine **RESP** calculates the residual of the volume equation (47), given by:

$$(r_v)_{ijk} = V_{ijk}^B - [V_{ijk}^A + \Delta t \sum_\alpha (uA)_\alpha^B].$$

The quantities V_{ijk}^B and $(uA)_\alpha^B$ are obtained by substituting $(p_v)_{ijk}$, the current approximation to the pressure p , into the linearized equation of state (48) and the cell face velocity equation (46). Note that before calling **RESP** the quantity $\bar{x}_i = x_i + s_i$ is formed, in order to compute the modified residual \bar{r}_i which is required in our modified Omin algorithm.

The subroutine **DRDP** computes the reciprocals of the diagonal elements of the implicitly defined matrix A to use as the preconditioner C . Whenever application by C is required, the array holding the diagonal elements of C is applied component-wise to the appropriate vector.

The remainder of the code implements the Omin algorithm for PCR as in-line scalar and vector operations, matching the logic of the algorithm in the right box of Figure 5. The stopping criterion employed is a point-wise test of the magnitudes of the components of the residual against a tolerance $\epsilon = 10^{-10}$ times the cell volume, or:

$$\|(r_v)_{ijk}\| \leq \epsilon V_{ijk}^A.$$

The subroutines **TSOLVE** and **VSOLVE** implement PCR for the solution of the implicit temperature and velocity equations, respectively. The algorithm used in each case is also based on the modified Omin algorithm in the right box of Figure 5, and the logic in each subroutine is very similar in form to that described above for the **PSOLVE** subroutine. In both cases, however, only a single equation is involved, and the logic and code simplify accordingly.

The following “key to the code” will enable a user to read some of the code and map it to the abstract modified Omin algorithm above. In the **PSOLVE** subroutine, the preconditioner C is represented by the array **rdrdp**. The modified residual \bar{r}_i is (usually) placed in the array **res**, whereas the normal residual r_i is (usually) placed in the array **resold**. The solution vector x_i , representing the corrected pressures, is placed in the array **p**, and the direction vectors p_i are kept in the array **dp**. Finally, the array **dres** is used to hold the vector Ap_i . With this key, it is not difficult to follow the code and map the logic to the modified version of the Omin algorithm appearing in the right box of Figure 5.

7 Summary and Conclusions

In §2 and §3 of this report, we presented a brief introduction to continuum mechanics, fluid mechanics, and the mechanics of chemically reactive fluids with sprays. Following this introduction, we took a close look in §4 at the governing equations of KIVA-II, which were more complex than the standard combustion equations due to the use of a turbulence model. The discretization procedures employed in KIVA-II were discussed in §5, including the ALE-finite volume spatial discretization, and the use of variably implicit time discretization schemes. We also outlined in detail the three phases of a single time step: the chemistry and droplet calculations of Phase A, the fluid diffusion and droplet velocity calculations of Phase B, and the fluid advection and mesh rezoning of Phase C. Finally, the most time-consuming parts of the simulation, the Phase B implicit diffusion calculations, were discussed in §6, including the forms of all discrete equations employed in Phase B, given in full detail. We also gave a short discussion of the use of the conjugate residual method, as employed in KIVA-II, for solution of the implicit equations.

Before ending this set of notes, we present and then discuss the implications of some performance statistics for one time step of a sample engine simulation, just to give an indication of which phases of the computation performed in KIVA-II are most time-consuming on sequential computers. Since our understanding of the inner workings of the KIVA-II code (or even the proper settings of the multitude of user-defined parameters) is still quite primitive at the time of this writing, these statistics should be taken only as an indication of what might be expected in a real simulation.

7.1 Cray Y-MP and SUN SPARC versions of KIVA-II

We have modified the original Cray version of KIVA-II in such a way as to enable execution on a SUN SPARC workstation. Therefore, we will present timings for both a SUN SPARC and one processor of a four processor Cray Y-MP.

Table 1 gives the total execution time required on each machine for one time step, broken down into various parts of the implicit Phase B solution. Table 2 presents these same timings as percentages of the total solution time. Finally, Table 3 presents the timings as percentages of the implicit solve time. These timing percentages agree with experiments published in [38].

Table 1: Total CPU seconds spent in various phases for a single time step.

Machine	Phase					
	Momentum Equations	Temperature Equation	Pressure Equation	Implicit Solution	All Other Phases	Total Solve
SUN SPARC	0.86	3.62	57.1	61.9	44.1	106
Cray Y-MP	0.05	0.40	5.00	5.47	3.39	8.86

Table 2: Percentage of total execution time spent in various phases.

Machine	Percent of Total Solve Time				
	Momentum Equations	Temperature Equation	Pressure Equation	Implicit Solution	All Other Phases
SUN SPARC	1	3	54	58	42
Cray Y-MP	1	4	56	62	38

From these tables, and from the timings published in [38], it is clear that most of the solution time is spent in the implicit Phase B solution; in particular, in the computation of the corrected pressure. In fact,

Table 3: Percentage of implicit solve time spent in various phases.

Machine	Percent of Implicit Solve Time		
	Momentum Equations	Temperature Equation	Pressure Equation
SUN SPARC	1	6	93
Cray Y-MP	1	7	92

some simple experiments indicate that as the mesh dimensions grow, the percentage of total solution time spent in the implicit pressure solution grows rapidly.

Unless the solution behavior is such that stability restrictions force the advection phase to become highly computationally intensive, it may happen that the complexity of the implicit solution phase will dominate as the mesh size grows. For model problems in three-dimensions, preconditioned conjugate gradient methods have complexity $O(N^{1.17})$. While the explicit portions of the computation must be performed with much smaller time steps due to the Courant stability limit, each step has $O(N)$ complexity. Which computation will dominate as the mesh size grows is not clear.

7.2 Other options for the implicit solves: multilevel methods

With regard to sequential efficiency, it may be possible to replace the conjugate residual iterative solution techniques with more efficient methods, namely multigrid or multilevel methods. It can be proven rigorously that multilevel methods have optimal $O(N)$ complexity for a large class of problems [9, 18], and their use for the solution of the elliptic equations arising at each time step during implicit solution of parabolic equations has been considered for example in [12, 22].

The arbitrary Lagrangian-Eulerian mesh may appear to preclude the use of a multigrid method, due to the difficulty in defining a coarse mesh. However, techniques for constructing coarse meshes from exactly these types of fine meshes have been considered in [13].

7.3 Parallel computing and KIVA-II

Some attempts have been made to implement KIVA-II on a distributed memory computer [38]. This work, which focussed on parallelizing the implicit portions of the Phase B solution on an Intel iPSC/860 super-computer, achieved mixed results.

The explicit portions of the computation in KIVA-II and related codes are trivially parallelizable; the computations performed at each time step require only “nearest-neighbor” communication, although many time steps may be required due to the Courant stability limit.

For the implicit solution procedures, however, the situation is more complex. The basic (unpreconditioned) Krylov subspace methods, such as the conjugate gradient and conjugate residual methods, require only matrix-vector products, inner products, and other vector-vector computations. These operations parallelize and vectorize quite easily, especially for arbitrary Lagrangian-Eulerian meshes in which each mesh point is connected in a regular fashion to the same fixed number of neighboring mesh points, regardless of how distorted the moving mesh becomes.

However, preconditioners are usually required to attain adequate convergence rates for Krylov methods, and unfortunately, it is generally the case that the better the preconditioner is, the more difficult it is to parallelize. Exceptions to this rule appear to be the multilevel and domain decomposition preconditioners [11], although their formulation requires a finite-element framework, and their value in practical numerical fluid mechanics has not been established.

7.4 Parallel multilevel methods

In the case of classical multigrid methods, while they may attain $O(N)$ sequential complexity in certain situations, they face their own set of problems on parallel computers. If massively parallel computers are used, then for a suitably coarse mesh, there are more processors than mesh points, causing processors to become idle. Even before this happens, the communication costs may begin to dominate the computation costs on coarse meshes.

All is not lost, however, as parallel multilevel algorithms have been designed to avoid exactly these problems; see [35] for an excellent discussion, and an application of some of these methods to the two-dimensional Euler equations. We note, however, that the seriousness of these problems with regard to multigrid efficiency on parallel computers, as well as the effectiveness of the new parallel multilevel algorithms, has been under debate recently; see for example [17] for a discussion and analysis.

In any event, multilevel methods, in some form, may prove useful for solution of the KIVA-II Phase B implicit equations on a massively parallel computer.

References

- [1] W. F. AMES, *Numerical Methods for Partial Differential Equations*, Academic Press, New York, NY, 1977.
- [2] A. A. AMSDEN, T. D. BUTLER, P. J. O'ROURKE, AND J. D. RAMSHAW, *KIVA: A comprehensive model for 2D and 3D engine simulations*, Tech. Rep. 850554, SAE, 1985.
- [3] A. A. AMSDEN, P. J. O'ROURKE, AND T. D. BUTLER, *KIVA-II: A computer program for chemically reactive flows with sprays*, Tech. Rep. LA-11560-MS, Los Alamos National Laboratory, 1989.
- [4] A. A. AMSDEN, J. D. RAMSHAW, L. D. CLOUTMAN, AND P. J. O'ROURKE, *Improvements and extensions to the KIVA computer program*, Tech. Rep. LA-10534-MS, Los Alamos National Laboratory, 1985.
- [5] A. A. AMSDEN, J. D. RAMSHAW, P. J. O'ROURKE, AND J. K. DUKOWICZ, *KIVA: A computer program for two- and three-dimensional fluid flows with chemical reactions and fuel sprays*, Tech. Rep. LA-10245-MS, Los Alamos National Laboratory, 1985.
- [6] D. A. ANDERSON, J. C. TANNEHILL, AND R. H. PLETCHER, *Computational Fluid Mechanics and Heat Transfer*, Hemisphere Publishing, New York, NY, 1984.
- [7] R. ARIS, *Vectors, Tensors, and the Basic Equations of Fluid Mechanics*, Dover Publications, New York, NY, 1962.
- [8] S. F. ASHBY, T. A. MANTEUFFEL, AND P. E. SAYLOR, *A taxonomy for conjugate gradient methods*, SIAM J. Numer. Anal., 27 (1990), pp. 1542–1568.
- [9] R. E. BANK AND T. F. DUPONT, *An optimal order process for solving finite element equations*, Math. Comp., 36 (1981), pp. 35–51.
- [10] A. I. BORISENKO AND I. E. TARAPOV, *Vector and Tensor Analysis with Applications*, Dover Publications, New York, NY, 1968.
- [11] J. H. BRAMBLE, J. E. PASCIAK, AND J. XU, *Parallel multilevel preconditioners*, Math. Comp., 55 (1990), pp. 1–22.
- [12] A. BRANDT, *Multigrid techniques: 1984 guide with applications to fluid dynamics*, Tech. Rep. GMD-Studien Nr. 85, GMD, Bonn, 1984.
- [13] A. BRANDT, J. E. DENDY, JR., AND H. RUPPEL, *The multigrid method for semi-implicit hydrodynamics codes*, J. Comp. Phys., 34 (1980), pp. 348–370.
- [14] J. D. BUCKMASTER, *An introduction to combustion theory*, in *The Mathematics of Combustion*, J. D. Buckmaster, ed., SIAM, Philadelphia, PA, 1985, pp. 3–46.
- [15] ———, *The Mathematics of Combustion*, SIAM, Philadelphia, PA, 1985.
- [16] A. J. CHORIN AND J. E. MARSDEN, *A Mathematical Introduction to Fluid Mechanics*, Springer-Verlag, Berlin, Germany, 1990.
- [17] N. H. DECKER, *On the parallel efficiency of the Frederickson-McBryan multigrid algorithm*, Tech. Rep. NAS1-18605, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, 1990.
- [18] W. HACKBUSCH, *Multi-grid Methods and Applications*, Springer-Verlag, Berlin, Germany, 1985.
- [19] J. B. HEYWOOD, *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, NY, 1988.
- [20] C. HIRSCH, *Numerical Computation of Internal and External Flows*, John Wiley & Sons Ltd, New York, NY, 1988.
- [21] C. W. HIRT, A. A. AMSDEN, AND J. L. COOK, *An arbitrary Lagrangian-Eulerian computing method for all flow speeds*, J. Comp. Phys., 14 (1974), pp. 227–253.

- [22] M. HOLST AND F. SAIED, *Parallel performance of some multigrid solvers for three-dimensional parabolic equations*, Tech. Rep. UIUCDCS-R-91-1697, University of Illinois at Urbana-Champaign, 1991.
- [23] O. D. KELLOG, *Foundations of Potential Theory*, Dover Publications, New York, NY, 1953.
- [24] R. J. LEVEQUE, *Numerical Methods for Conservation Laws*, Birkhäuser Verlag, Berlin, Germany, 1990.
- [25] C. C. LIN AND L. A. SEGEL, *Mathematics Applied to Deterministic Problems in the Natural Sciences*, Macmillan Publishing Company, New York, NY, 1974.
- [26] P. J. O'ROURKE AND A. A. AMSDEN, *Implementation of a conjugate residual iteration in the KIVA computer program*, Tech. Rep. LA-10849-MS, Los Alamos National Laboratory, 1986.
- [27] J. D. RAMSHAW, *Partial chemical equilibrium in fluid dynamics*, Phys. Fluids, 23 (1980), pp. 675–680.
- [28] J. D. RAMSHAW, P. J. O'ROURKE, AND L. R. STEIN, J. Comp. Phys., 58 (1985).
- [29] W. RUDIN, *Principles of Mathematical Analysis*, McGraw-Hill, New York, NY, 1953.
- [30] L. A. SEGEL, *Mathematics Applied to Continuum Mechanics*, Dover Publications, New York, NY, 1977.
- [31] J. SERRIN, *Mathematical principles of classical fluid dynamics*, in Encyclopedia of Physics, vol. 13, Springer-Verlag, New York, NY, 1959.
- [32] T. M. SHIH, *Numerical Heat Transfer*, Hemisphere Publishing Corporation, New York, NY, 1984.
- [33] G. STRANG, *Introduction to Applied Mathematics*, Wellesley-Cambridge Press, Wellesley, MA, 1986.
- [34] R. TEMAM, *Navier-Stokes Equations*, North-Holland, New York, NY, 1977.
- [35] R. S. TUMINARO, *Multigrid Algorithms on Parallel Processing Systems*, PhD thesis, Dept. of Computer Science, Stanford University, 1989. Available as Report No. STAN-CS-90-1299.
- [36] R. S. VARGA, *Matrix Iterative Analysis*, Prentice-Hall, Englewood Cliffs, NJ, 1962.
- [37] F. A. WILLIAMS, Phys. Fluids, 1 (1958).
- [38] O. YASAR, B. GEBBEKEN, AND C. RUTLAND, *Parallelization of KIVA-II on iPSC/860 supercomputer*, tech. rep., College of Engineering, University of Wisconsin-Madison, 1992.