

Wasatch

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Wasatch is a finite volume computational fluid dynamics (CFD) code that employs the spatial operator (SpatialOps) and expression (ExprLib) libraries at its foundation. It is developed as a software component within the Uintah computational parallel framework. Wasatch provides the interface between the Uintah API and the various classes and tools supplied by the SpatialOps and ExprLib libraries making its development entirely based on the expressions graph abstraction.

Contents

| | | |
|----------|---|-----------|
| 1 | Capabilities | 4 |
| 1.1 | Momentum Transport | 4 |
| 1.2 | LES Modeling | 6 |
| 1.2.1 | Momentum Equations | 6 |
| 1.2.1.1 | Energy Equation:THIS SECTION REQUIRES REVISION . . . | 7 |
| 1.2.2 | Subgrid Closure | 7 |
| 1.3 | Generic Scalar Transport | 10 |
| 1.4 | Population Balances | 11 |
| 1.5 | Basic CFD Algorithm using Expression Graphs | 11 |
| 1.5.1 | Improved Boundary Conditions Support | 11 |
| 1.6 | Runge-Kutta Time Integrator | 12 |
| 2 | Order of Accuracy Verification | 13 |
| 2.1 | Order-of-Accuracy in a Single Dimension | 14 |
| 2.2 | Combined Spatio-Temporal Order-of-Accuracy Analysis | 15 |
| 2.3 | Verification of Wasatch | 15 |
| 3 | Scalability | 18 |
| 4 | Boundary Conditions | 19 |
| 4.1 | Overview of Defining Boundary Conditions | 19 |
| 4.2 | Scalar Transport Boundary Conditions | 20 |
| 4.3 | Fluid Flow Boundary Conditions | 20 |
| 4.3.1 | Inlets, Walls, and Moving Walls | 20 |
| 4.3.2 | Pressure Outlet | 21 |
| 5 | Modeling General Scalar Transport | 22 |
| 6 | Modeling Species Transport | 23 |
| 7 | Modeling Dispersed-Phase Flows | 24 |
| 7.1 | Precipitation | 24 |
| 7.1.1 | Governing Equations | 24 |
| 7.1.2 | Birth Models | 24 |
| 7.1.3 | Growth Models | 25 |

| | | |
|----------|---|-----------|
| 7.1.4 | Multi Environment Mixing Model | 25 |
| 8 | Summary of Current Capabilities and Work in Progress | 27 |

Chapter 1

Capabilities

Wasatch currently supports basic physical models of transport phenomena in fluids and gases. These may be reactive with variable density or non-reactive. The working model is based on writing expressions that reflect physical processes, akin to mathematical terms in a partial differential equation (PDE). These expressions are subsequently used in a variety of transport equations as needed. Transport equations are derived from a base class and each specializes in solving a particular class of problems. Currently, Wasatch supports the following transport equations:

- Generic scalar transport
- Momentum transport
- Population balances via moment transport

A wide range of expressions are currently implemented in Wasatch. These include the standard convective and diffusive fluxes as well as stresses. In addition, a variety of source terms.

1.1 Momentum Transport

Wasatch solves the variable density momentum equations

$$\frac{\partial \rho \mathbf{u}}{\partial t} = -\nabla \cdot \rho \mathbf{u} \mathbf{u} - \nabla \cdot \boldsymbol{\tau}_{ij} - \nabla p + \rho \mathbf{g} \quad (1.1)$$

in conjunction with the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \quad (1.2)$$

Here, ρ stands for the density, $\mathbf{u} = (u, v, w)$ is the velocity field, p is the pressure, \mathbf{g} is the gravity vector, and $\boldsymbol{\tau}_{ij}$ is the stress tensor given by

$$\tau_{ij} = -2\mu S_{ij} + \frac{2}{3}\mu \delta_{ij} S_{kk}; \quad S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (1.3)$$

The rate of strain tensor S_{ij} is a fundamental quantity when using gradient diffusion turbulence models and will be used extensively in subsequent sections.



Figure 1.1: Expression graph for a two dimensional fluid flow problem using the Poisson equation for the pressure.

The code supports central, upwind, and over ten flux limiters for the discretization of the convective flux. The pressure is resolved by solving the pressure Poisson equation. This is constructed by first taking the divergence of the momentum equations. Then the continuity equation is used to substitute for the temporal term in the resulting equation. At the outset, one recovers a Poisson equation for the pressure

$$\nabla^2 p = \frac{\partial^2 \rho}{\partial t^2} + \nabla \cdot \nabla \cdot \rho \mathbf{u} \mathbf{u} - \nabla \cdot \nabla \cdot \tau_{ij} - \nabla \cdot \rho \mathbf{g} \quad (1.4)$$

The solution of Eq. (1.4) requires the inversion of a linear system of equations. At the time of writing, Wasatch can solve the constant density momentum equations in three dimensions with periodic boundary conditions. The solution is based on the expressions graph showing that a basic CFD algorithm may be achieved using the graph based algorithm approach. A sample graph for a two dimensional fluid flow is shown in Fig. 1.1.

Pressure Projection Wasatch uses the Pressure-Poisson-Equation (PPE) formulation to handle the pressure-velocity couple. The PPE formulation consists of first taking the divergence of the momentum equations and substituting the continuity equation to yield a Poisson equation for the pressure. This version of the pressure projection provides an elegant and straight-forward equation for the pressure. Part of the difficulty of using the PPE formulation resides in the specification of appropriate boundary and initial conditions. While boundary conditions correspond to “natural” conditions imposed on physical quantities such as mass flowrate, pressure gradient, and velocity; specification of the initial conditions requires further attention on the Pressure poisson equation.

Constant Density For a constant density flow, the Pressure-Poisson-Equation reduces to

$$\nabla^2 p = \nabla \cdot \nabla \cdot \rho \mathbf{u} \mathbf{u} - \nabla \cdot \nabla \cdot \tau_{ij} - \nabla \cdot \rho \mathbf{g} \quad (1.5)$$

1.2 LES Modeling

Wasatch uses Favre filtering as the basis for its LES approach. Favre filtering is defined as a density-weighted filtering operation to accomodate variable density. It is given by the following operation

$$\overline{\rho\phi} = \bar{\rho}\widetilde{\phi} \quad (1.6)$$

where the overbar denotes a traditional filtering operation. A traditional filtering operation consists of a convolution of a transported variable (i.e. a variable that one wishes to filter) with a filter. This is written as

$$\bar{\phi} = \int_{\Omega} G(\mathbf{r})\phi(\mathbf{x} - \mathbf{r}) d\mathbf{r} \quad (1.7)$$

1.2.1 Momentum Equations

To make further headway, we apply the traditional filter to the governing fluid transport equations. Starting with continuity, we have

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot \bar{\rho}\mathbf{u} = 0 \quad (1.8)$$

Then, one makes use of the Favre filtering operation by setting $\bar{\rho}\mathbf{u} = \bar{\rho}\widetilde{\mathbf{u}}$. At the outset, the Favre-filtered continuity equation is given by

$$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot \bar{\rho}\widetilde{\mathbf{u}} = 0 \quad (1.9)$$

Moving on to the momentum equation, the filtering operation yields

$$\frac{\partial \bar{\rho}\mathbf{u}}{\partial t} = -\nabla \cdot \bar{\rho}\mathbf{u}\mathbf{u} - \nabla \cdot \bar{\tau}_{ij} - \nabla \bar{p} + \bar{\rho}\mathbf{g} \quad (1.10)$$

It is best to transform to Favre filtering term-by-term

- $\frac{\partial \bar{\rho}\mathbf{u}}{\partial t} = \frac{\partial \bar{\rho}\widetilde{\mathbf{u}}}{\partial t}$
- $\nabla \cdot \bar{\rho}\mathbf{u}\mathbf{u} = \nabla \cdot \bar{\rho}\widetilde{\mathbf{u}}\mathbf{u} = \nabla \cdot \bar{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}} + (\nabla \cdot \bar{\rho}\widetilde{\mathbf{u}}\mathbf{u} - \nabla \cdot \bar{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}}) \equiv \nabla \cdot \bar{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}} + \nabla \cdot \tau_{ij}^R; \quad \tau_{ij}^R \equiv \bar{\rho}\widetilde{\mathbf{u}}\mathbf{u} - \bar{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}}$
- $\nabla \cdot \bar{\tau}_{ij} = \nabla \cdot \widetilde{\tau}_{ij} + (\nabla \cdot \bar{\tau}_{ij} - \nabla \cdot \widetilde{\tau}_{ij}) \equiv \nabla \cdot \widetilde{\tau}_{ij} + \nabla \cdot \tau_{ij}^L$
- $\bar{\rho}\mathbf{g} = \bar{\rho}\mathbf{g}$

where τ_{ij}^R and τ_{ij}^L are subgrid-scale stress tensors (SGS) that result from applying filtering to the convective and diffusive terms in the momentum equations. At the outset, the filtered momentum equations may be written as

$$\frac{\partial \bar{\rho}\widetilde{\mathbf{u}}}{\partial t} = -\nabla \cdot \bar{\rho}\widetilde{\mathbf{u}}\widetilde{\mathbf{u}} - \nabla \cdot \widetilde{\tau}_{ij} - \nabla \bar{p} - \nabla \cdot \tau_{ij}^R - \nabla \cdot \underbrace{\tau_{ij}^L}_{\text{neglect}} + \bar{\rho}\mathbf{g} \quad (1.11)$$

It is evident from Eq. (1.11) that both subgrid tensors τ_{ij}^R and τ_{ij}^L require closure. However, it may be argued that the subgrid tensor τ_{ij}^L resulting from viscous stresses is negligible compared to τ_{ij}^R that results from filtering of the convective terms [Geurts et al., 1993, Vreman et al., 1995].

1.2.1.1 Energy Equation: THIS SECTION REQUIRES REVISION

The filtered energy equation is

$$C_v \frac{\partial \bar{\rho} \tilde{T}}{\partial t} + C_v \frac{\partial}{\partial x_k} (\bar{\rho} \tilde{v}_k \tilde{T}) = -\bar{p} \frac{\partial \tilde{v}_k}{\partial x_k} + \tilde{\sigma}_{ik} \frac{\partial \tilde{v}_k}{\partial x_l} + \frac{\partial}{\partial x_k} \left(\tilde{\kappa} \frac{\partial \tilde{T}}{\partial x_l} \right) - C_v \frac{\partial q_k}{\partial x_k} \quad (1.12)$$

Similarly for the filtered energy equation, the diffusive term needs to be modeled somehow. Again, by considering eddy viscosity SGS model we can obtain

$$q_k = -\frac{\bar{\rho} v_T}{Pr_t} \frac{\partial \tilde{T}}{\partial x_k} \quad (1.13)$$

Where $v_T = C\Delta^2 |\tilde{S}|$ and Pr number is again parametrized using dynamic models to obtain

$$Pr_t = C \left\langle \hat{\rho} \hat{\Delta}^2 |\hat{S}| \frac{\partial \hat{T}}{\partial x_k} \frac{\partial \tilde{T}}{\partial x_k} - \Delta^2 \bar{\rho} |\tilde{S}| \frac{\partial \tilde{T}}{\partial x_k} \frac{\partial \tilde{T}}{\partial x_k} \right\rangle \times \left\langle \left(\frac{1}{\hat{\rho}} \widehat{\bar{\rho} \tilde{v}_k \tilde{T}} - \widehat{\bar{\rho} \tilde{v}_k} \tilde{T} \right) \frac{\partial \tilde{T}}{\partial x_k} \right\rangle^{-1} \quad (1.14)$$

1.2.2 Subgrid Closure

The most common approach to modeling the subgrid-scale tensors is based on eddy-viscosity models. First proposed by [Smagorinsky, 1963], these have the general form

$$\tau_{ij}^R = \underbrace{\tau_{ij}^d - \frac{1}{3} \delta_{ij} \tau_{kk}^d}_{\text{deviatoric}} + \underbrace{\frac{1}{3} \delta_{ij} \tau_{kk}^d}_{\text{isotropic}} \quad (1.15)$$

The deviatoric subgrid-stress tensor τ_{ij}^d is modeled as

$$\tau_{ij}^d = 2\mu_t \left(\tilde{S}_{ij} - \frac{1}{3} \delta_{ij} \tilde{S}_{kk} \right) \quad (1.16)$$

where μ_t is the eddy- or turbulent-viscosity and \tilde{S}_{ij} is the Favre-filtered rate of strain - a computable quantity.

The isotropic subgrid-stress tensor τ_{ij}^s may be absorbed into the filtered pressure or entirely neglected [Erlebacher et al., 1992, Garnier et al., 2009]. This is based on the observation that small scales are generally incompressible [Garnier et al., 2009]. In fact, τ_{kk} may be written in terms of the subgrid Mach number as

$$\tau_{kk} = \gamma M_{\text{sgs}}^2 \bar{p} \quad (1.17)$$

where γ is the ratio of specific heats and M_{sgs} is the subgrid Mach number whose values is expected to be small when the turbulent Mach number of the large scales is low.

Upon substitution of Eq. (1.15) into Eq. (1.11) one recovers

$$\frac{\partial \bar{\rho} \tilde{\mathbf{u}}}{\partial t} = -\nabla \cdot \bar{\rho} \tilde{\mathbf{u}} \tilde{\mathbf{u}} - \nabla \cdot \tilde{\boldsymbol{\tau}}_{ij} - \nabla \bar{p} - \nabla \cdot \boldsymbol{\tau}_{ij}^d + \bar{\rho} \mathbf{g} \quad (1.18)$$

Given that all quantities – except ν_t – are computable, the essence of all eddy-viscosity models is then to model the turbulent viscosity ν_t .

Constant Smagorinsky-Lilly Model In the constant Smagorinsky-Lilly model, a simple algebraic relation is proposed for the eddy-viscosity [Smagorinsky, 1963]. This form may be written as

$$\mu_t = \bar{\rho} (C_s \Delta)^2 |\tilde{S}| = \bar{\rho} L_s^2 |\tilde{S}|$$

where C_s is a constant, Δ is an average measure of the cell size, usually taken as the average cell volume $V^{1/3}$, and $|\tilde{S}| = \sqrt{2\tilde{S}_{ij}\tilde{S}_{ij}}$. Also, L_s is commonly referred to as the mixing length and is a measure of the characteristic mixing length of turbulent eddies.

In Wasatch, we implement a variant of Smagorinsky’s classic model. To allow users to fine-tune the turbulent viscosity based on physical input, we introduce a lengthscale to the calculation of the smagorinsky mixing length. The desired features of our model are

- As the grid spacing Δ approaches the kolmogorov scale, the turbulent viscosity should approach zero since all scales are resolved.
- As the grid spacing drifts from the kolmogorov scale, the effect of mixing due to small scales becomes more pronounced and hence the turbulent viscosity increases.
- Ability to recover constant smagorinsky model when desirable.

These features may be accomplished by setting

$$L_s = C_s \Delta \left(1 - \frac{\Delta}{\eta}\right) \quad (1.19)$$

Here, C_s is a scaling constant that is *not* equal to the Smagorinsky constant and η is a characteristic small scale of the problem. Typically, η may be taken as the Kolmogorov scale. It may be evaluated from the following scaling law

$$\frac{L}{\eta} \sim \text{Re}^{3/4} \quad (1.20)$$

where L is a characteristic length of the large scale eddies and Re is the Reynolds number of the flow. For example, for the flow in a pipe of diameter D , the characteristic length may be taken as $L = D$ while $\text{Re} = \frac{\rho V D}{\mu}$. The behavior of Eq. (1.19) is shown in Fig. 1.2. Two key regimes may be identified in this figure. The first lies at $0 < \eta < \Delta$ (to the left of $\eta = \Delta$ mark) designates the region where the mesh spacing is larger than the small scales. Hence, as the mesh spacing becomes larger than the small scales (i.e. only very large scales are resolved), more dissipation must be added to mimic the dissipation caused by the small scales. The second regime lies in the region $\Delta < \eta < \infty$ and is only included for mathematical completion. This region indicates that the mesh size is smaller than the smallest scales and is not truly part of an LES model. Its inclusion, however, is necessary to recover the Smagorinsky classic model as $\eta \rightarrow \infty$.

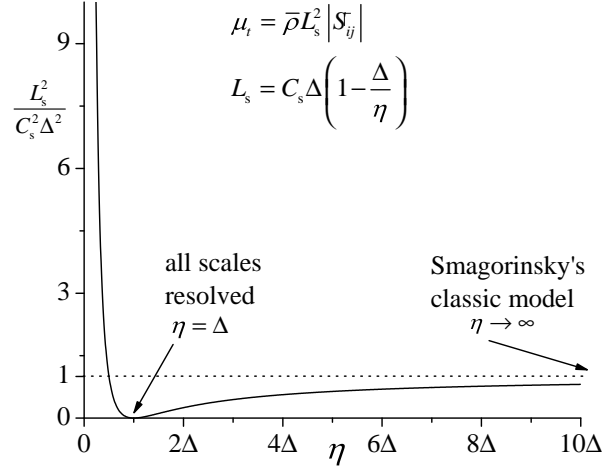


Figure 1.2: Behavior of the mixing length in the modified Smagorinsky model used in Wasatch.

Dynamic Smagorinsky Model The most important difference between filtered and non-filtered momentum equation is in the diffusive term, τ_{kl} . According to the Smagorinsky eddy viscosity model it can be modeled as

$$\tau_{kl} - \frac{1}{3}q^2\delta_{kl} = -2C\bar{\rho}\Delta^2|\tilde{S}|(\tilde{S}_{kl} - \frac{1}{3}\tilde{S}_{mm}\delta_{kl}) \quad (1.21)$$

where $\tilde{S}_{kl} = \frac{1}{2}(\partial\tilde{u}_k/\partial x_l + \partial\tilde{u}_l/\partial x_k)$, $|\tilde{S}| = (2\tilde{S}_{kl}\tilde{S}_{kl})^{1/2}$ and $q^2 = \tau_{ii}$. q^2 is also parameterized using Yoshizawa's model to obtain

$$q^2 = 2C_I\bar{\rho}\Delta^2|\tilde{S}|^2 \quad (1.22)$$

Where Δ is the grid size.

C and C_I are Smagorinsky constants which can be assumed to be a fixed number and also can be calculated using dynamic models. By using dynamic models and applying test-filters these constants are parameterized as

$$C_I = \frac{\langle \widehat{\bar{\rho}\tilde{v}_k\tilde{v}_k} - (1/\hat{\bar{\rho}})(\widehat{\bar{\rho}\tilde{v}_k})(\widehat{\bar{\rho}\tilde{v}_k}) \rangle}{\langle 2\hat{\bar{\rho}}\hat{\Delta}^2|\hat{\tilde{S}}|^2 - 2\Delta^2\bar{\rho}|\tilde{S}|^2 \rangle} \quad (1.23)$$

$$C = \frac{\left\langle [\widehat{\bar{\rho}\tilde{v}_k\tilde{v}_l} - (1/\hat{\bar{\rho}})(\widehat{\bar{\rho}\tilde{v}_k}\widehat{\bar{\rho}\tilde{v}_l})]\tilde{S}_{kl} - \frac{1}{3}\tilde{S}_{mm}(\mathcal{T}_{jj} - \hat{\tau}_{jj}) \right\rangle}{\left\langle -2\hat{\bar{\rho}}\hat{\Delta}^2|\hat{\tilde{S}}|(\hat{\tilde{S}}_{kl}\tilde{S}_{kl} - \frac{1}{3}\hat{\tilde{S}}_{mm}\tilde{S}_{jj}) + 2\Delta^2(\bar{\rho}|\tilde{S}|\tilde{S}_{kl}\tilde{S}_{kl} - \frac{1}{3}\bar{\rho}|\tilde{S}|\tilde{S}_{mm}\tilde{S}_{jj}) \right\rangle} \quad (1.24)$$

Where $\langle \rangle$ indicates volume averaging and $\mathcal{T}_{jj} - \hat{\tau}_{jj} = \mathcal{L}_{jj} = \widehat{\bar{\rho}\tilde{v}_j\tilde{v}_j} - (1/\hat{\bar{\rho}})(\widehat{\bar{\rho}\tilde{v}_j})(\widehat{\bar{\rho}\tilde{v}_j})$ and over hat means the test filter is applied.

Wall-Adapting Local Eddy-Viscosity (WALE) In the WALE model [Geurts et al., 1993], the eddy-viscosity is modeled as

$$\mu_t = \rho (C_w\Delta)^2 \frac{(S_{ij}^d S_{ij}^d)^{3/2}}{(\tilde{S}_{ij}\tilde{S}_{ij})^{5/2} + (S_{ij}^d S_{ij}^d)^{5/4}} \quad (1.25)$$

Here, C_w is the WALE model constant, Δ is the average cell size, and S_{ij}^d is the traceless symmetric part of the square of the velocity gradient tensor, given by [Nicoud and Ducros, 1999]

$$S_{ij}^d = \frac{1}{2} (g_{ij}^2 + g_{ji}^2) - \frac{1}{3} \delta_{ij} g_{kk}^2; \quad g_{ij}^2 = g_{ik} g_{kj}; \quad g_{ij} = \frac{\partial u_i}{\partial x_j} \quad (1.26)$$

Care must be taken in evaluating the components of S_{ij}^d .

1.3 Generic Scalar Transport

Wasatch can solve any scalar transport equation of the general form

$$\frac{\partial \rho \phi}{\partial t} = -\nabla \cdot \rho \phi \mathbf{u} + \nabla \cdot \rho \Gamma_\phi \nabla \phi + S_\phi \quad (1.27)$$

This general form is basically the strong form of the scalar transport equation when density is variable. Wasatch has the capability of choosing between the strong form or the weak form of this transport equation. Density type can also be specified in the input files of wasatch to determine if it is constant or variable. Regarding these capabilities we can have three more possible forms of transport equations rather than 1.27. Those forms are:

Strong form with constant density

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot \phi \mathbf{u} + \nabla \cdot \Gamma_\phi \nabla \phi + \frac{S_\phi}{\rho} \quad (1.28)$$

Weak form with variable density

$$\frac{\partial \phi}{\partial t} = -\mathbf{u} \cdot \nabla \phi + \frac{1}{\rho} \nabla \cdot \rho \Gamma_\phi \nabla \phi + \frac{S_\phi}{\rho} \quad (1.29)$$

Weak form with constant density

$$\frac{\partial \phi}{\partial t} = -\mathbf{u} \cdot \nabla \phi + \nabla \cdot \Gamma_\phi \nabla \phi + \frac{S_\phi}{\rho} \quad (1.30)$$

Wasatch can now solve transport equations in strong form with either constant or variable density. Solving the weak form of the equation has not been implemented yet and is in progress.

The main reason that wasatch keeps both strong and weak form is to compare their result in future to see which one is more beneficial. In strong form with variable density wasatch solves for, $\rho \phi$, and in order to update the for scalar variable we need to solve a nonlinear equation where, $\rho \phi$ and $\rho = F(\phi)$ are given, in order to find the scalar variable in the current time step. On the other hand, weak form has its own problems. For example to solve weak form equations' convective terms in order to apply limiters on this term this equation is used

$$\mathbf{u} \cdot \nabla \phi = \nabla \cdot \phi \mathbf{u} - \phi \nabla \cdot \mathbf{u} \quad (1.31)$$

And limiters can be used on the terms on the RHS easily. The scalar variable in this case should be assumed to be approximately constant in each cell on the grid.

1.4 Population Balances

Wasatch currently supports a basic population balance equation with a single internal coordinate. The targeted equation is written as

$$\frac{\partial N}{\partial t} = -\nabla \cdot \mathbf{u}N + \frac{\partial gN}{\partial r} + b; \quad N \equiv N(\mathbf{x}, r, t) \quad (1.32)$$

where r is an internal coordinate, $g \equiv \frac{dr}{dt}$ denotes the growth rate of r , and b represents the death/birth rates of particles. To make further headway, solution of the population balance equation is usually achieved by solving for the moments of the number density function, N . The k^{th} moment is defined as

$$m_k \equiv \int_{-\infty}^{+\infty} r^k N(\mathbf{x}, r, t) dr \quad (1.33)$$

By applying the moment transformation to 1.32, we recover the moment transport equation

$$\frac{\partial m_k}{\partial t} = -\nabla \cdot \mathbf{u}m_k - k \int_{-\infty}^{+\infty} r^{k-1} gN dr + \int_{-\infty}^{+\infty} r^k b dr \equiv F(m_{k+i}); \quad i \in \mathbb{Q} \quad (1.34)$$

The right-hand-side (RHS) in Eq. (1.34) may be a function of any moment order. As such, we can write additional transport equations for these moments. However, one usually ends up with a several moments that require closure. This may be achieved by the quadrature method of moments.

The quadrature method of moments (QMOM) is a closure technique used to solve the moment transport equations for population balance problems with a single internal coordinate. The technique is based on Gaussian quadrature to achieve closure for the unknown moments. Subsequently, the quadrature nodes and abscissae are obtained using the lower order moments by using the product-difference algorithm. The product-difference algorithm incurs a series of recursion formulas that result in an eigenvalue problem whose solution yields the abscissae (eigenvalues) and weights (eigenvectors).

We recently implemented the moment transport equation in Wasatch with the flexibility to solve for any number of moments. We also added three growth rate models; namely, constant growth, mono-surface nucleation, and bulk diffusion to illustrate the ease with which new growth models can be implemented.

1.5 Basic CFD Algorithm using Expression Graphs

Wasatch is currently able to solve the momentum equations in three dimensional space with periodic boundary conditions using the graph-based algorithm. An example problem that uses two dimensional

1.5.1 Improved Boundary Conditions Support

We have recently revisited the boundary conditions processing in Wasatch. The user/developer has the flexibility of automatically specifying Dirichlet or Neumann boundary conditions on any field type (Scalar, Staggered) and any expression used in the solution process. Furthermore, the

boundary condition functionality is now fully templated on the type of field. This allows for partial and full specialization for fields that require specific treatment such as normal stresses.

1.6 Runge-Kutta Time Integrator

There is currently a working version of a third order, strong stability preserving Runge-Kutta integrator. There are two problems to be resolved as of this writing, one pertaining to the pressure projection on multi-patch problems while the other has to do with field memory management at various integrator stages. An abstraction for multistage integrators is in order to address these problems as well as provide support for higher order time integrators in the future.

Chapter 2

Order of Accuracy Verification

Order-of-accuracy analysis is based on the concept that the error must be reduced as spatial and temporal steps are reduced. By comparing the errors at different grid levels, one can estimate the theoretical order of accuracy for a code. First, we review the general concept.

The order of accuracy of a discretization method is defined as *the exponent of the leading order term in the total error* incurred by the discretization process. The total error refers to the accumulation of truncation and round off errors throughout the spatial and temporal domains. It can be generally defined as

$$E = |\phi_{\text{exact}} - \phi_{\text{numerical}}| \quad (2.1)$$

where ϕ_{exact} and $\phi_{\text{numerical}}$ refer to the exact and numerical solutions, respectively.

Round-off errors are those due to finite precision calculation on a computer while the truncation error represents the error induced by neglecting terms in a finite numerical approximation. For most practical purposes, one can neglect round-off errors and focus on how the truncation error is propagated throughout the solution domain. This is the strategy that we will adopt in this document.

To illustrate how the truncation error is estimated, we make use of Taylor series expansions to approximate the various differential terms in an equation. For example, for a transported scalar ϕ on a grid with uniform spacing Δx , the Taylor series at an arbitrary point i is written as

$$\phi_{i+1} = \phi_i + \frac{d\phi_i}{dx} \Delta x + \frac{d^2\phi_i}{dx^2} \frac{\Delta x^2}{2!} + \frac{d^3\phi_i}{dx^3} \frac{\Delta x^3}{3!} + \dots \quad (2.2)$$

One can then approximate the first derivative at grid point i via

$$\frac{d\phi_i}{dx} = \frac{\phi_{i+1} - \phi_i}{\Delta x} + \underbrace{\frac{d^2\phi_i}{dx^2} \frac{\Delta x}{2!} + \frac{d^3\phi_i}{dx^3} \frac{\Delta x^2}{3!} + \dots}_{\text{truncation error}} \quad (2.3)$$

Then, one can choose to approximate the first derivative by using the first term on the right-hand-side of the previous equation. The remaining terms are then known as the truncation error. The truncation error has to satisfy certain properties for a discretization scheme to be consistent. For example, all terms in the truncation error must decrease monotonically. Furthermore, the coefficients in the truncation error must be bounded.

The truncation error is usually lumped into a single term and assigned the \mathcal{O} terminology

$$T.E. = \mathcal{O}(\Delta x^m), \quad m \in \mathbb{R}^+ \quad (2.4)$$

This definition has a precise meaning: as $\Delta x \rightarrow 0$, the truncation error is proportional to Δx^p with a proportionality constant that is independent of Δx . Alternatively, one can write

$$\lim_{\Delta x \rightarrow 0} \frac{T.E.}{\Delta x^m} = M \quad (2.5)$$

where M is a constant. Then, the truncation error can be written as

$$T.E. = M\Delta x^m \quad (2.6)$$

Subsequently, and by neglecting round-off errors, the total error consists of the accumulated truncation error when discretization is carried out throughout the spatial or temporal domain. In general, this is not the sum of the truncation error incurred by applying a discretization method at a single point. We will discuss how the truncation error accumulates shortly, but for the moment, the total error can be written as

$$E = \alpha\Delta x^p \quad (2.7)$$

where α is a real constant that is independent of the mesh size while p is a positive real number that designates the order-of-accuracy of a discretization method. The purpose of an order-of-accuracy verification is to determine the exponent p in the total error induced by the discretization process.

2.1 Order-of-Accuracy in a Single Dimension

To solve for p in Eq. (2.7), one needs two equations. With knowledge of an exact solution, a test problem can be setup and solved on two different grid spacings, Δx_1 and $\Delta x_2 = \frac{\Delta x_1}{r_x}$. Then, one calculates the errors associated with these two grids. These are given by

$$\begin{cases} E_1 = \alpha\Delta x_1^p \\ E_2 = \alpha\Delta x_2^p \end{cases} \quad (2.8)$$

These equations can be easily solved by taking the difference of their logarithms. One recovers

$$\ln E_1 - \ln E_2 = p \ln \Delta x_1 - p \ln \Delta x_2 \quad (2.9)$$

or

$$\ln \frac{E_1}{E_2} = p \ln \frac{\Delta x_1}{\Delta x_2} = p \ln r_x \quad (2.10)$$

finally, the observed order of accuracy is at hand

$$p = \frac{\ln \frac{E_1}{E_2}}{\ln r_x} \quad (2.11)$$

A word of caution must be said about temporal order of accuracy analysis. Many people think that by taking

It is easiest to first determine the temporal order of accuracy of a transient CFD code. As discussed in the previous paragraph

2.2 Combined Spatio-Temporal Order-of-Accuracy Analysis

Without loss of generality, the truncation error may be represented as

$$E = u_{\text{exact}} - u_{\text{numerical}} = \alpha \Delta t^p + \beta \Delta x^q + \gamma \Delta y^r + \delta \Delta z^s \quad (2.12)$$

This excludes all terms that have mixed orders in them.

2.3 Verification of Wasatch

Temporal Order of Accuracy Wasatch currently entertains both forward Euler (FE) and 3rd order Runge-Kutta strong stability preserving (RK3SSP) time integrators. To verify the temporal order of accuracy of these integrators, an ODE test was designed. In the first, we solve an ODE with a time dependent source term. Care must be taken when calculating the order of accuracy at the first time-step. In this scenario, the observed order of accuracy will be one order higher than the theoretical one. This can be shown as follows. Consider a time-stepping discretization of order p . This solves the following ODE

$$\frac{d\phi}{dt} = L(\phi) \quad (2.13)$$

written in discretized form, this leads to

Time-Dependent Source Term Our choice falls upon

$$\frac{d\phi}{dt} = \sin t; \quad \phi(0) = -1 \quad (2.14)$$

The analytical solution for this case is

$$\phi_{\text{exact}} = -\cos t \quad (2.15)$$

The tests varied over a time interval of 1 second with systematic mesh refinement. The results for both the FE and the RK3SSP are shown in the table below

Implicit Source Term In this verification test, we solve the following ODE

$$\frac{d\phi}{dt} = \phi; \quad \phi(0) = 1 \quad (2.16)$$

Since this is an ODE, the spatial resolution is set to [2, 2, 2] in Wasatch. The code is run with both FE and RK3 time integrators at several time-steps ranging from

Table 2.1: Observed temporal order of accuracy using $\frac{d\phi}{dt} = \sin t$. Results are taken at $t = 1$ s with systematic timestep refinement.

| | Forward Euler | | RK3SSP | |
|------------|------------------------|----------------|-------------------------|----------------|
| Δt | $E = \Phi - \phi $ | Observed Order | $E = \Phi - \phi $ | Observed Order |
| 0.1 | 4.245×10^{-1} | | 1.596×10^{-8} | |
| 0.05 | 2.113×10^{-1} | 1.006 | 9.976×10^{-10} | 4.000 |
| 0.025 | 1.054×10^{-1} | 1.003 | 6.623×10^{-11} | 4.000 |
| 0.0125 | 5.265×10^{-2} | 1.001 | 3.900×10^{-12} | 3.998 |
| 0.00625 | 2.631×10^{-2} | 1.000 | 2.508×10^{-13} | 3.959 |
| 0.003125 | 1.315×10^{-2} | 1.000 | 3.175×10^{-14} | 2.984 |

Table 2.2: Observed temporal order of accuracy using $\frac{d\phi}{dt} = \phi$. Results are taken at $t = 2$ s with systematic timestep refinement.

| | Forward Euler | | RK3SSP | |
|------------|------------------------|----------------|------------------------|----------------|
| Δt | $E = \Phi - \phi $ | Observed Order | $E = \Phi - \phi $ | Observed Order |
| 0.1 | 6.615×10^{-1} | | 5.684×10^{-4} | |
| 0.05 | 3.491×10^{-1} | 0.922 | 7.395×10^{-5} | 2.942 |
| 0.025 | 1.795×10^{-1} | 0.959 | 9.431×10^{-6} | 2.971 |
| 0.0125 | 9.103×10^{-2} | 0.979 | 1.191×10^{-6} | 2.985 |
| 0.00625 | 4.584×10^{-2} | 0.989 | 1.496×10^{-7} | 2.992 |
| 0.003125 | 2.301×10^{-3} | 0.994 | 1.874×10^{-8} | 2.996 |
| 0.0015625 | 1.152×10^{-3} | 0.977 | 2.346×10^{-9} | 2.997 |

Table 2.3: Observed spatial order of accuracy using Taylor-Vortex. Results are taken at $t = 2s$ with systematic time-step refinement.

| | u | | v | |
|------------|--------------------------|----------------|--------------------------|----------------|
| Δx | $E = \text{norm}(U - u)$ | Observed Order | $E = \text{norm}(U - u)$ | Observed Order |
| 0.1257 | 1.856×10^{-3} | | 1.856×10^{-3} | |
| 0.0628 | 4.650×10^{-4} | 1.997 | 4.650×10^{-4} | 1.997 |
| 0.0314 | 1.163×10^{-4} | 1.999 | 1.163×10^{-4} | 1.999 |
| 0.0157 | 2.908×10^{-5} | 2.000 | 2.908×10^{-5} | 2.000 |

Spatial Order of Accuracy A method of manufactured solution has been done on wasatch using forward Euler method on a Taylor-Vortex problem to check the spatial and temporal order of accuracy. We state the spatial order of accuracy here as long as the temporal order of accuracy has been already shown in this document in previous subsection.

In order to check the spatial order of accuracy we looked at the four different grid resolutions for our domain, and we chose 0.001, 0.0005, 0.00025 and 0.000125 respectively for their time step. However, we just looked at the results after the first time step. This is in order to neglecting the temporal accuracy in the explicit solvers. Because, those terms will be calculated in the previous time step, therefore, in all of our cases they will be calculated at time zero. So, because of using the same time for these terms we don't let the time accuracy to influence our results for grid convergence study

Taylor-Vortex problem is a 2D problem where the exact solutions are:

$$u(x, y, t) = 1 - A \cos(x - t) \sin(y - t) \exp(-2vt) \quad (2.17)$$

$$v(x, y, t) = 1 + A \sin(x - t) \cos(y - t) \exp(-2vt) \quad (2.18)$$

Where in this study, $A = 4$ and $v = 0.1$.

In order to calculate the error the norm over the whole area is taken to obtain

$$E = \text{norm}(u_{\text{exact}} - u_{\text{numerical}}) \quad (2.19)$$

So we can consider all of the point on the grid together.

Results for Spatial order of accuracy The results for both u and v using the FE are shown in the table below

As it is clear from the table the spatial order of accuracy is 2 as it was expected for the FE method with central 3 point discretization in space.

Chapter 3

Scalability

To test some scalability aspects of Wasatch, we implemented the model discussed in Eq. (??).
[DEVIN, can you add some results here?]

Chapter 4

Boundary Conditions

4.1 Overview of Defining Boundary Conditions

Wasatch provides the machinery to apply Dirichlet and Neumann boundary conditions. Our approach is based on setting boundary conditions on ghost cells at the boundaries of the computational domain to reproduce the desired boundary at the face. This is illustrated in Fig. 4.1.

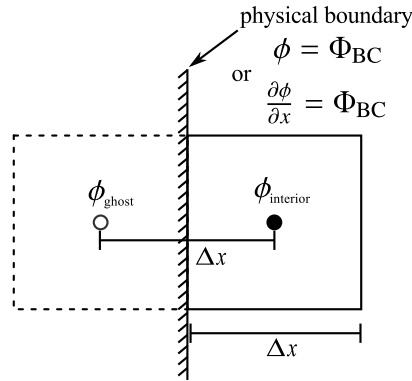


Figure 4.1: Boundary condition specification in Wasatch. Here, Φ_{BC} designates the desired value of the scalar or its flux at the boundary, ϕ_{interior} is the interior value of the scalar, and ϕ_{ghost} is the ghost value to be set.

Mathematically, this may be written as follows. Consider a scalar ϕ for which a boundary condition is to be specified. The ghost value of ϕ may then be written as

$$\phi_{\text{ghost}} = \alpha \phi_{\text{interior}} + \beta \Phi_{\text{BC}} \quad (4.1)$$

where α and β are real coefficients that depend on the type of boundary condition specified. These are summarized in Table 4.1 .

For Staggered fields on uniform structured grids, a simplification follows for setting Dirichlet conditions. In this case, certain boundary faces coincide with staggered control volumes and the desired Dirichlet condition may be set directly on those cells.

| | α | β |
|-----------|----------|-------------|
| Dirichlet | 0.5 | 0.5 |
| Neumann | 1.0 | $-\Delta x$ |

Table 4.1: Summary of coefficients for setting values at ghost cells to reproduce a desired boundary condition at a physical boundary.

4.2 Scalar Transport Boundary Conditions

The treatment of scalar boundary conditions follows from the previous discussion. Specification of either fixed values or fluxes of transported scalars is easily achieved using the machinery discussed in §4.1.

4.3 Fluid Flow Boundary Conditions

4.3.1 Inlets, Walls, and Moving Walls

Inlets and walls, whether moving or stationary, share the same type boundary conditions. The user specifies the momentum at those boundaries. Treatment of the pressure is derived from the pressure Poisson equation as follows. For simplicity, we illustrate this in one-dimension at a boundary cell on the x-minus side of the computational domain. In this case, the pressure poisson equation is written as

$$\frac{\partial^2 p}{\partial x^2} = \frac{\partial F}{\partial x} \quad (4.2)$$

Using second order finite differencing, Eq. (4.2) may be written as

$$\frac{p_{-1} - 2p_0 + p_1}{\Delta x^2} = \frac{F_{1/2} - F_{-1/2}}{\Delta x} \quad (4.3)$$

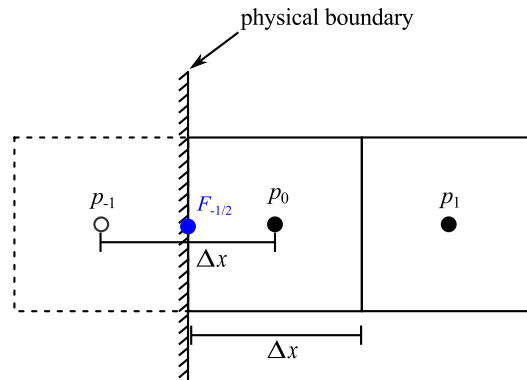


Figure 4.2: Derivation of pressure boundary conditions.

Here, both p_{-1} and $F_{i-\frac{1}{2}}$ are unknown and one may be inclined to specify these quantities at the boundary. However, by using the x -momentum equation, one can relate these quantities as follows. On an x -minus cell, the x -momentum equation may be written as

$$\left(\frac{\partial \rho u}{\partial t}\right)_{-\frac{1}{2}} = -\left(\frac{\partial p}{\partial x}\right)_{-\frac{1}{2}} - F_{-\frac{1}{2}} \quad (4.4)$$

Again, using central finite differencing, one recovers

$$\left(\frac{\partial \rho u}{\partial t}\right)_{-\frac{1}{2}} = -\frac{p_0 - p_{-1}}{\Delta x} - F_{i-\frac{1}{2}} \quad (4.5)$$

or

$$\frac{p_{-1} - p_0}{\Delta x} = \left(\frac{\partial \rho u}{\partial t}\right)_{-\frac{1}{2}} + F_{i-\frac{1}{2}} \quad (4.6)$$

Both the pressure coefficient matrix and the pressure right-hand-side are modified accordingly. For practicaly reasons, we set the $F_{-\frac{1}{2}} = 0$ on faces perpendicular to momentum directions.

4.3.2 Pressure Outlet

Chapter 5

Modeling General Scalar Transport

Chapter 6

Modeling Species Transport

Chapter 7

Modeling Dispersed-Phase Flows

7.1 Precipitation

Wasatch supports precipitation-physics reactions utilizing the quadrature method of moments to solve the population balance equation. The internal coordinate in this case is the particle radius.

7.1.1 Governing Equations

The precipitation model utilized in Wasatch uses the implemented moment transport equations.

$$\frac{\partial m_k}{\partial t} = -\nabla \cdot \mathbf{u}m_k - k \int_{-\infty}^{+\infty} r^{k-1} gN \, dr + \int_{-\infty}^{+\infty} r^k b \, dr \equiv F(m_{k+i}); \quad i \in \mathbb{Q} \quad (7.1)$$

with QMOM used as closure for the moments. The moments that require closure will change based on the growth rate model that is utilized, and the closure is taken care of automatically in the Wasatch algorithm. The relevant terms dictating the reaction rate are tabulated by the extent of reaction and the mixture fraction. The main term required is the supersaturation value of the liquid. The source term for the reaction progress is

$$S_\xi = \frac{1}{\iota} \sum_{\alpha=1}^n \nu_\alpha S_{3,\alpha} \quad (7.2)$$

where $S_{3,\alpha}$ is the source term of the third moment, representing the volume, of species α , ν_α is the molecular volume, and ι is the maximum moles of precipitate.

7.1.2 Birth Models

Nucleation terms in Wasatch can be specified as one of three distributions, point, uniform, and normal. Each of these distributions requires the specification of a nucleation radius which can either be set as a constant or as the critical radius $r^* = r_0 / \log(S)$. The uniform and normal distributions also require a specified standard deviation for the distribution. The coefficient used for the birth term can either be set as constant or using the classical nucleation definition

$$B_0 = \text{Exp}\left[\frac{16\pi}{3} \left(\frac{\gamma}{K_B T}\right)^3 \frac{v}{N_A \log(S)^2}\right] \quad (7.3)$$

where γ is the surface energy, K_B is the Boltzman constant, T is the temperature in Kelvin, v is the molecular volume, and N_A is Avogadro's constant. The Wasatch formulation also includes a “pre-Birth coefficient” which is used as a conversion factor from SI units into smaller lengths (μm or nm) used as precipitate measurements.

7.1.3 Growth Models

Currently Wasatch has three growth models implemented; constant growth, bulk diffusion and monosurface nucleation. Each model uses a different form of $g(r)$ with $g(r) = g_0$, $g(r) = g_0 \frac{1}{r}$, and $g(r) = g_0 r^2$, respectively, as well as a different requirement for the closure of the moment transport equations as: none, m_{-2} & m_{-1} , and m_{k+1} . The bulk diffusion model uses the appropriate coefficient as

$$g_0 = vDC_{eq}(S - \bar{S}) \quad (7.4)$$

with D as the diffusion coefficient, C_{eq} as the equilibrium concentration and where \bar{S} can either be set as one, or set as needed for Ostwald Ripening as

$$\bar{S} = \exp(2v\gamma/RT) \quad (7.5)$$

For Ostwald ripening, the r appearing in the exponential does not allow for this term to be converted into a moment of the problem, therefore the quadrature weights and abscissae are used to evaluate the Ostwald ripening term. For monosurface nucleation the growth coefficient is

$$g_0 = \beta_A D d^3 \exp(-\Delta G/K_B T) \quad (7.6)$$

with

$$\Delta G = \frac{\beta_L \gamma^2 d^2}{4\beta_A K_B T \log(S)} \quad (7.7)$$

where β_L and β_A are shape factors, and d is the molecular diameter. As with the birth models, a “pre-Growth coefficient” can be used for unit conversions.

7.1.4 Multi Environment Mixing Model

Wasatch has a subgrid scale model for mixing for the precipitation flows. Since the source terms of the moment transport equations are highly dependent on the current value of the moments, which are solved on the slow scale, a tabulation of data for use in a continuous PDF (i.e. such as a flamelet) is not a viable option. Instead a discrete PDF is used consisting of three delta functions, one at mixture fraction $z = 0$, one at mixture fraction $z = 1$, and the third at the average mixture fraction. In precipitation flows, no reaction occurs at either mixture fraction 0 or 1, so only the source terms from the central delta function need to be solved.

Wasatch requires the averaged mixture fraction and the scalar variance to be solved on the grid. Then the weights of the three delta functions are calculated as

$$w_1 = \frac{\langle z'^2 \rangle}{\langle z \rangle} \quad (7.8)$$

$$w_2 = \frac{\langle z'^2 \rangle - \langle z \rangle + \langle z \rangle^2}{\langle z \rangle^2 - \langle z \rangle} \quad (7.9)$$

$$w_3 = \frac{-\langle z'^2 \rangle}{\langle z \rangle - 1} \quad (7.10)$$

where $\langle z \rangle$ is the average mixture fraction, and $\langle z'^2 \rangle$ is the scalar variance.

When the Multi Environment Model is enabled, the moment equations are only solved for the second environment with the moments from environments 1 and 3 held constant. The averaged moments are then post-processed based on the values of the environment weights. In addition the transport of the second environment requires a new source term to account for the change in the moments due to mixing.

$$S_{\phi_{\alpha,2}, mix} = -\frac{dw_1/dt}{w_2}(\phi_{\alpha,1} - \phi_{\alpha,2}) - \frac{dw_3/dt}{w_2}(\phi_{\alpha,3} - \phi_{\alpha,2}) \quad (7.11)$$

Where $\phi_{\alpha,i}$ represents the α th precipitate moment located in the i th mixing environment. With the time derivatives of the weights of the mixing environments calculated as

$$\frac{dw_1}{dt} = \frac{-\langle \epsilon_\phi \rangle}{\langle z \rangle} \quad (7.12)$$

$$\frac{dw_3}{dt} = \frac{-\langle \epsilon_\phi \rangle}{1 - \langle z \rangle} \quad (7.13)$$

where $\langle \epsilon_\phi \rangle$ is the scalar dissipation rate.

Chapter 8

Summary of Current Capabilities and Work in Progress

Table 8.1: Synopsis of Wasatch development.

| Task | Status |
|---|-------------|
| Advective terms including flux limiters | completed |
| Diffusive terms for basic diffusive flux expressions | completed |
| Tabular property evaluation for implementation of common combustion models | completed |
| Pressure projection | completed |
| Basic CFD algorithm using expressions graph | completed |
| Boundary conditions for scalar transport | completed |
| Quadrature method of moments | completed |
| Basic population balance equation | completed |
| Filter operator for dynamic turbulent models | completed |
| Boundary conditions for momentum equations | in progress |
| Weak form of transport equations | in progress |
| Variable density algorithm (including appropriate terms in the pressure projection) | in progress |
| Higher-order time integrator (Runge-Kutta based) | in progress |
| LES models for turbulent diffusive fluxes (Smagorinsky and dynamic models) | in progress |

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