**Applied Simulation of Flow, Transport, Reactions, and Deformation**

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**Chapter 1 Overview**

**Motive**

A broad range of scientific and engineering problems involve interactions between flowing fluid, transport of heat and mass, reactions between chemical and biota, and deformation of solids. Each of these topics covers a huge body of information, described in myriad books and presented in many courses. Indeed, many of the disciplines within engineering and science cover these topics in their own unique way, creating a broad diversity in perspective. The great depth and variety of treatment of these topics reflects their importance and provides a strong basis for applications in specific disciplines. Environmental engineers need to know how fluids flow and reactions occur in anaerobic digesters in order to improve designs, whereas hydrogeologists need to understand fluid flow and transport through porous media in order to test hypotheses about natural degradation of contaminants. In many cases, fluency in these domain-specific applications is a requirement for professional competency.

Processes of flow, transport, reactions and deformation are indeed diverse, but they share a common thread that helps to unify their understanding. Analyses of those techniques are based on conservation principles, and the equations governing them follow from a single, generic conservation equation. This provides a unifying strategy for developing a basic understanding because one approach can be adapted to many applications.

The similarity in governing equations was recognized by computer scientists who developed a class of numerical models capable of simulating a remarkable diversity of processes. These so-called “multiphysics” packages offer the capability to simulate myriad processes within a single software package. This was an important advance because it provided a tool for simulations that appeared to be only limited by the imagination of the user. It held the potential to streamline the testing of new ideas and evaluation of new designs, providing a catalyst for innovation and insight.

There is a catch, of course. Multiphysics software is a remarkable tool, but it is only a tool. Anyone who has worked in a woodshop knows that the same tool that produces a masterpiece can also produce a useless scrap. It is the skill of the craftsman that makes the difference.

These notes were motivated by the goal of improving simulation craftsmanship. The topics will be limited to flow, transport, reactions and deformation, and the intent will be to improve general understanding of how these processes behave. Examples drawn from specific domains in engineering and science will be used as the basis for numerical experiments, which will hopefully build intuitive understanding and illustrate methods that can be applied elsewhere.

**Strategy**

Simulations use a strategy that goes from an initial concept to the communication of results

**Conceptual Model**

It is impossible to simulate reality. Real processes nearly all involve interactions of atoms or molecules and computers are too small to simulate all the atoms in a region of interest. Moreover, real geometries are often extremely intricate and it is impossible to measure all the geometric details. Imagine, for example, if you wanted to simulate flow of oil through a sand bed by representing the interconnected network of pores in the sand. It is currently possible to measure the geometry of pores in sand using devices developed for medical imaging, so you could get started. But you can only analyze a modest-sized sample, so you would be unable to measure all the pores in an oil reservoir, and even if you could, computers are too small to represent that much information.

*Contiuum*

Fortunately, there are ways to simplify reality so the essence is retained while the details are avoided. The strategy is to make assumptions that allow the complex to be simplified enough to be adequately represented. One important assumption involves lumping atoms and molecules together into continuous fluids or solids. Interactions between the molecules are represented using effective properties, like the viscosity of a fluid or the elastic modulus of a solid, so the individual molecules can be ignored. This assumption allows a materials to be viewed as a continuum. One consequence of the continuum assumption is that it places a lower limit on the size of a region that can be simulated. Clearly, the continuum assumption would be inappropriate for problems spanning regions the size of an individual molecule. Regions large enough to contain many molecules are needed justify the assumption of a continuum—the lower size limit is a matter of debate and will depend on details of a particular problem.

*Essential details*

Most of the processes considered in these notes will assume materials can be represented as continua. This is an important first step in defining an analysis, but additional simplification is always needed. This involves identifying the essential details of geometries and processes necessary to define a problem. The strategy is often to simplify the problem as much as possible while it still retains important characteristics of the original. Nearly all problems can be simplified this way, and there is often a wide range of simplification that can be done.

The simplified version of reality is a *conceptual model*. It can be described in text and illustrations, and the conceptual model captures an essence of the problem. In general, the conceptual model defines spatial and temporal aspects, processes, and parameters:

1. Spatial: number of spatial dimensions and configuration or geometry of the domain

2. Temporal: whether the important variables change with time or are steady

3. Processes: what the important processes are, where they occur, how they interact with each other, and what variables are needed to characterize them.

 4. Parameters: what the important material properties are, their values, and how they are distributed.

*Evolution of the conceptual model*

The conceptual model will serve as the basis for the simulation and as such it is a key component of the analytical tool we will use to learn about a process. A useful strategy for understanding complicated problems is to develop a conceptual model with several levels of simplification. The simplest version may be too simple to address all the complexities of the problem, but it can address some important aspects and provide a foundation for more complicated models that follow.

Here are some general guidelines for developing an initial conceptual model:

Spatial:

* Use domains with simple shapes. Rectangles or circles can approximate many much more complicated geometries.
* Use the lowest possible dimension. Pose the problem in 1D if possible and then expand to 2D or 3D as needed.

Temporal:

* Assume the problem is at steady state, if possible. In many cases, the steady state result will serve as the initial condition for a transient problem.

Processes:

* Assume the simplest processes that could represent the problem.
* Avoid coupling of multiple processes.
* Avoid parameters that change during the analysis.
* Assume laminar flow instead of turbulent, and single phase fluids instead of multiple phases.

Parameters:

* Assume parameters are uniformly distributed within domains.

Once a baseline conceptual is identified, the task is to make it incrementally more complicated by relaxing the simplifying assumptions.

**Translate Concept**

The conceptual model is usually a simplified, qualitative description of a problem and it serves as the basis for the numerical model. Translating the conceptual model into a numerical model that can be analyzed to provide quantitative results requires the following steps.

*Geometry*

Define the size and shape of the region that will be analyzed. The overall geometry will consist of

*Subdomains* are areas in 2D problems and volumes in 3D. Geometries can consist of multiple subdomains.

*Edges* are lines. Subdomains in 1D will consist of edges.

*Points* are points in all dimensions.

*Governing Equations*

Identify the governing equations based on the processes that need to be considered. Governing equations will be based on conservation principles and will typically be in the form of a differential equation. The first step in this process is to identify the quantity that is conserved and the *dependent* variable in the problem.

The conservation principle is typically applied to a control volume and three components are identified to satisfy the requirements of conservation

1. Flux
2. Storage
3. Source

Each of these components is written in terms of the dependent variable and then combined to form a governing equation.

Governing equations typically include parameters*.* These parameters result from the different components used in the conservation analysis. For example, the flux component may introduce a parameter, such as the diffusion constant, that relates flux to a gradient in the dependent variable.

Simplifications from the conceptual model are used to tailor governing equations to a particular problem. For example, fluid flow assumed to be in the laminar regime would be simulated using a governing equation that differs from the equation used if the flow was turbulent.

Some problems require multiple dependent variables and multiple governing equations that are coupled together. For example, analyzing a transport problem may require an equation to govern fluid flow with pressure or head as the dependent variable, and another governing equation governing transport with concentration as the dependent variable.

*Boundary Conditions*

The behavior of the dependent variables on the boundaries is described using boundary conditions. A boundary condition for each dependent variable on each external boundary is required, as a minimum. Some problems involve internal boundaries.

Boundary conditions take the form of equations. Parameters may be introduced to describe processes on boundaries.

*Parameters*

Parameters are used to scale the response to particular effect. Many parameters are material properties. In simple problems, parameters are the same everywhere, they are *uniform*, and they are unchanged with time, they are *constant*. Note that uniform and constant are often used interchangeably, but it is convenient to be able to clearly distinguish things that change with time from things that change spatially.

Parameters may change as a result of things that happen during an analysis. Material properties, like density, may change as a result of heating, for example. *Constitutive* equations describe how a parameter may change during a process.

*Time*

Some problems involve processes that vary spatially, but are fixed in time. These processes are at steady state, and they are called *stationary*. Processes that change with time are called transient, or *time dependent*.

*Initial Conditions*

Transient problems require specifying values of the dependent variable at the start of the simulation.

*Discretize using mesh or grid*

Numerical simulations involve converting a governing differential equation into an approximate form that is valid over a mesh or grid covering the geometry. The result of the simulation will depend to some extent on the mesh that is used. In some cases, a poorly designed mesh may cause large errors in the results, or it may prevent the analysis from reaching a solution. This may occur when the mesh is too coarse, for example. Meshes that are very fine may result in a simulation that is so time consuming to solve that it is of little practical value.

Meshes consist of *elements* that typically have simple shapes. The simplest shape is a triangle in 2D and tetrahedron in 3D, but rectangles or quadrilaterals are also commonly used. The vertices of the elements are called nodes.

**Solve**

The solution process involves representing the governing equation in discrete form on each of the elements. This results in many equations that are assembled in a matrix. Specialized mathematical techniques have been developed to solve the resulting matrix to obtain values of the dependent variables over the mesh as a function of time. These values are the results.

**Interpreting Results**

Solving the problem is obviously important, but there are typically some additional steps required to interpret the results.

*Tablulate data*

Tables of numbers are sometimes all that is needed for an interpretation. For example, if you are verifying that your numerical solution matches an exact result, then you may want to know the values predicted by both solutions at certain times and places. It will be important to obtain tabulated data for this application.

*Graphical rendering*

Most interpretations will be facilitated by rendering results graphically. x-y plots can be used to show how a dependent variable changes with time at a particular point, a time series plot. They also can show how the variable changes with space at a particular time, a profile plot. These are 1D plots.

2D plots show how a variable is distributed and they typically involve contours or coloring to show different values.

3D plots show 3 spatial dimensions. Isosurfaces in 3D are the equivalent of 2D contour lines.

Variables also change with time. It is often convenient to plot 1D profiles taken from different times to show how a variable varies with time. This is cumbersome in 2D and 3D, however. In those cases, one option is to create a video that shows how the 2D or 3D distribution changes with time.

Becoming fluent in graphical rendering will be an important skill in interpreting the results of your analyses.

*Parameter sensitivity*

Understanding how a variable changes with a parameter value can lead to important insights. For example, suppose that you want to know how changes in pressure affect the steady flow rate of a fluid draining by gravity through a conduit. Both the viscosity and the density of the fluid change with temperature, and these changes will affect the flow rate. In this case, you would solve the problem and determine the flow rate for one temperature, then repeat for many other temperatures. This is a parameter sweep, where you sweep through many values of temperature. Ultimately, you would plot flow rate as a function of temperature. It may be difficult to anticipate how temperature affects this process, so the results of this plot will help to train your intuition.

Conducting and interpreting parameter sweeps will be important to understanding some types of problems.

*Parameter estimation*

Some problems involve using a model to interpret data. On application is to adjust the model to match data obtained experimentally. This is a common way of estimating parameters, for example.

The general process of parameter estimation starts with developing a model that represents the system of interest and that can predict the variable that was measured experimentally. This is called the forward model. The forward model is run and the results are compared to experimental data. The value of one or more parameters is varied and the process is repeated in an effort to minimize the error between the observed and predicted values. In simple cases, you may be able to run a parameter sweep and plot the error between predicted and observed as a function of the parameter value. The minimum value of the error could show up on this plot. Many problems involve multiple parameters and it is impractical to estimate them using a parameter sweep. In these cases, there are a variety of numerical methods that can be used to control the execution of the forward model in order to identify a set of parameters that gives results that best match data.

*Engineering design*

Models play an important role in designing something that works. Calculations have always been an important aspect of design, but until recently calculations were only able to account for very idealized cases, the simplest of conceptual models. Complexities that were important to a design had to be evaluated using prototypes. In some cases, the prototypes could be scaled down in size using appropriate scaling laws. Design options were evaluated by building multiple prototypes.

This strategy can be effective, but building and testing prototypes is expensive so you various design details were often evaluated by building prototypes and seeing what happens. In some cases, you may set up a model to simulate a baseline design, and then make adjustments to understand how the parameters control performance. This could help train your intuition, but it also may be used to identify an optimal design with the best performance. The dimensions of the baseline design could be a controlling parameter sUsing models to facilitate design is another application where you would run a forward model multiple times. In this case, you would have some specifications that you want to meet and there would be some aspects of the design that could be adjusted in order to meet those specs.

**Communicate Results**

There is an old saying that asks whether a tree falling in the woods makes a sound if no one can hear it. You could ask the same question about whether an analysis is relevant if no one can read about it. Indeed, your analyses will only be of value if you can communicate what you did. In general, when you communicate about an analysis it is worthwhile to consider including

Motive: What is the background that makes the problem you are solving interesting?

Objectives: What are you trying to accomplish with the analysis?

Method: How did you accomplish the objectives?

Results: What did you find when you used the methods?

Conclusions: What can you conclude from what you found?

**Scope**

The notes cover topics in fluid flow, chemical reactions, transport of mass and heat, and deformation of solids. I will refer to these topics broadly as “reactive transport.” The specific topics that will be covered include

**Flow**

 Porous media

 Laminar

 Turbulent

 Multi-phase

**Reactions**

 Chemical

 Biological

 Surface reactions

**Transport**

 Diffusion and osmosis

 Advection and dispersion

 Reactions and transport

 Heat transport

 Variable density flow

**Deformation**

 Elasticity

 Poroelasticity

**Governing Equations**

There is a long list of equations governing the processes covered in these notes, and they all follow from one simple equation describing the concept of conservation of some quantity over a control volume. This generic conservation equation only contains three terms, yet it is the basis for the more specific, and in many cases more complicated, equations used to describe processes of fluid flow, transport and deformation.

Conservation laws follow from the principle that certain basic quantities can be tracked through a control volume. Mass, momentum, energy, and electrical charge are examples of these basic quantities. The rate of transport of the quantities into the control volume plus the rate at which the quantity is produced equals the rate of transport out plus the rate of change of the quantity stored inside the control volume.

The strategy taken in the following section is to develop the generic conservation equation first, and then show how equations governing other processes follow from this common concept.

**Flux**

Transport processes will be described in terms of flux, which will always be used here to mean a quantity moving through a unit area in a unit time. Introducing  as a generic quantity that is being conserved, flux is written in terms of basic units as

  (1)

where *L* and *T* are basic units of length and time. Later *M* will be used for basic units of mass. Square brackets will be used to denote units. The subscript *c* means that the length is taken along the control volume. *f* can take the form of mass flux, momentum flux, energy flux, for example. Flux is a vector quantity, so the magnitude of the vector has units given above, and it is implied that *L*c is measured normal to the direction of the vector.

It will be convenient to express the amount of  per unit volume in the control volume, so introducing

  (2)

The concentration of a chemical, or density of a material are examples of *c*. It is important to recognize that *c* is taken over the entire control volume. We will need to adjust (2) if we want *c* to represent the concentration of a compound dissolved in water in a porous material because the concentration is expressed per unit volume of water and only a fraction of the control volume contains water.

There are two basic mechanisms by which quantities can be transported, and they differ in the role of fluid flow. One mechanism, **D**, involves flux without fluid flow and the other, **A,** relies on flow. Diffusion of mass or conduction of heat are examples of **D**, and advection is an example of a flux that relies on flow. Advective flux is typically given by

  (3)

where **q**is the volumetric flux of the material containing The bold font means that the **q** and **A** are vectors The units of **q** are

  (4)

where *L3*f is a volume of the moving material, typically a fluid, and *L*2c is a cross-sectional area of the control volume normal the flux direction, *T* is time. Here we have intentionally separated the length scales associated with the fluid and the control volume to consider cases where the fluid occupies a fraction of the control volume.

**Source**

The quantity may be produced or consumed by a process operating within the control volume. A chemical reaction could be the source of a chemical or heat energy, for example. The effect of a source will be characterized by the rate of change of  caused by the process per unit volume, *V*, so

  (5)

**Storage change**

The amount of storedin the control volume will change with time, and this change is the essence of a problem that is transient. The amount of  in a differential volume is *c**V,* so storage change will be characterized by the rate of change, (d*c*/dt)*V*

**Application using an infinitesimal control volume**

A straightforward way to obtain the conservation law is to apply the principle to an infinitesimal control volume of dimensions x, y, z. Recall that the principle is: *The rate of transport of the quantities into the control volume plus the rate at which the quantity is produced equals the rate of transport out plus the rate of change of the quantity inside the control volume.*

*z*



S

**D**in*yz* + **A**in*yz* 

*y*

*x*

|  |
| --- |
| Figure 1. Schematic of processes associated with conservation over a control volume.  |

The terms on the left represent rates of input of  by the fluxes **D** and **A**, and the terms on the right are output rates of also represented by fluxes. The differential control volume is *V*=*x**y**z*. Apply the conservation principle using the quantities in Figure 1 gives

 

Dividing by the volume of the control volume, xyz, and cancelling terms gives

 

The advective term, A, is given by eq (3), so substituting gives

  (6)

The analysis above only considered fluxes in one direction, but in general the fluxes can be in 3D, so (6) becomes

 

where the subscript (e.g. *q*n) is the component of the vector in the *n* direction.

Recall that the nabla operator is . When applied to a scalar field, like temperature, , gives the gradient. However, when applied to a vector, the nabla operator gives the divergence of the vector. Using the volumetric flux vector, **q** as an example

 

where *q*n is the component of the vector in the *n* direction.

**The General Conservation Law**

All the major processes of interest to this course are governed by a generic conservation law that follows from (6) using the divergence operator

  (7a)

or

  (7b)

The dependent variable is *c*, the quantity of interest per unit volume. The term on the left side of the equation, S, is a source term, and the first term on the right side is the divergence of the flux. The last term is the rate of change of the quantity stored per unit volume. An even more compact way to write the conservation equation is

  (7c)

where advection and diffusion have been combined in a general flux.



**General Conservation Law in Integral Form**

The expression outlined above is straightforward to visualize when applied to an infinitesimally small control volume. But if the control volume is somewhat larger, then we might expect *J*, *S* and *c* to vary spatially across the control volume. We can still use the conservation principle, but we need to sum the contributions from the different terms. In this case, we describe the conservation concept as:

*The rate of total a quantity in across the boundaries equals the rate of change of storage plus the rate of a quantity is produced.*

We will assume a control volume of arbitrary volume, *V*c and surface area, *A*c.

*Flux across the boundaries*

The input rate across a unit area of boundary is the product of the inward flux normal to the boundary and a unit area. Now do this over the entire surface area of the control volume. Summing the contribution from each unit area gives the total net rate moving across the boundary, *Q*in. This can be determined by integrating the flux normal to the boundary over the surface area, *A*c, of the control volume

  (8a)

where **n** is a unit vector normal to the boundary pointing outward, so is the flux out of the control volume normal to the boundary. The negative sign appears because the normal vector is outward and we are interested in an inward flux.

*Sources*

The rate of production of  from sources, *Q*sourse, within an infinitesimal control volume is given in (5) as S*d*V. Now, if we assume a control volume of finite size where S varies, then to total production from the source is

  (8b)

*Storage change*

The rate of change of the total quantity stored is

  (8c)

Combining the three terms (8) gives the integral form of the conservation law applied to a control volume

 - (9)

Net rate in from flux across Rate of change of storage

boundary

 Rate produced by an internal source

Equation (9) and eq (7c) are both expressions of the conservation law. This seems impossible because the two equations seem to share little in common. Here is how to see their equivalence. The Divergence Theorem says that

  (10)

The right side of (10) is the same as the first term in (9), so substituting



 The expression in the blue box involves volume integrals over the same region, so the integrands can be combined

  (11)

Eq (11) is satisfied if the expression in the square brackets is zero

 

Rearranging gives

 

which is the same as eq. 7c.

The mass conservation concept is expressed in differential form in eqs (7) and in integral form in (9). These equations are equivalent, but we will use the differential form (7) nearly exclusively in the following notes. This sacrifice to completeness is done in an effort to maintain consistency, which hopefully will improve clarity. The analysis of the governing equation will start with (7b). The integral form (9) and the divergence theorem (11) will be used again later in the notes to explain the finite element method.

**Example 1: Conservation of Mass, and Continuity**

Conservation of mass is expressed by using , and it follows that . Mass per unit volume can be interpreted as a *concentration* or *density*. Concentration is used when the mass being conserved is contained within another material, which occupies the control volume. Density is used when the mass being conserved is material that fills the control volume. The first case could be a concentration of a compound dissolved in water, for example, whereas the second case could consider the density of the water itself.

Assuming that mass of the quantity of interest fills the control volume gives , where the dependent variable  is densityIn this case, the mass can be transported across the boundaries of the control volume when flow is occurring, but no mass flux occurs if no flow occurs. So, **D**=0 and substituting into (3) gives

 **A***=***q** 

It is possible that mass could be added to the control volume, say by injection, so 

 S = M (13)

where M is the rate of mass produced by the source per unit volume. Substituting (12) and (13) into (7a) gives the mass conservation equation

  (14)

The continuity equation is generally written with M=0

  (15)

Mass conservation is a basic principle assumed in many processes.

**Example 2: Conservation of Mass During Transport**

Assuming that mass of the quantity of interest is contained within another material, designated by subscript *f*, within the control volume gives , where *C* the dependent variable is mass per unit volume *L*f3 of the other material. Using *n* allows the material *f* to only partly fill the control volume. Typically, the material *f* is a mobile fluid.

An example of this scenario is a compound dissolved in water in a porous material. In this case, the concentration *C* is expressed per unit volume of the pore water, and *n* is porosity

  (16)

The porous material is assumed to be saturated with water in this case.

Mass flux [M/(L2T)] in a static fluid occurs by diffusion and is given by

  (17)

where *D\** is the effective molecular diffusion coefficient for a porous media. 

Recalling that the volumetric flux of the fluid *f* is **q** , a component of the mass flux can occur with the fluid as **q***C* . Additional mass flux occurs by mechanical dispersion, so the total advective mass flux is

  (18)

The source term describes the rate of mass produced by a chemical reaction, injection, or other means

 S = *Rm* (19)

where *R* is the rate of mass produced per unit volume. Substituting (17) through (19) into (7a) gives the equation for mass transport by advection and dispersion

  (20)

The advection dispersion equation is commonly modified by factoring

  (21)

and introducing the hydrodynamic dispersion

  (22)

to get

  (23)

Further simplification is possible if the porosity, *n*, is constant (in time) and uniform (in space) because it can be taken out of the derivatives to give

  (24)

where the average linear velocity is

  (25)

**Example 3: Conservation of Heat Energy**

Conservation of heat energy is expressed by setting , and it follows that *c* is an energy density. . Considering energy in the form of heat, *c* = *c*p*T,* where *c*p is the heat capacity [E/(M] and *T* is temperature.

Note that ** in square brackets means units of time, whereas *T* elsewhere means temperature.  in square brackets means units of temperature.

Heat flux [E/(L2T)] when the fluid is static occurs by conduction and is given by

  (26)

where *K*h is the bulk thermal conductivity of the media.

A component of the heat flux can occur as convection with the flowing fluid as *q**c*p*T,* where  is the fluid density and *c*p is the fluid heat capacity, and recalling that the volumetric flux of the fluid *f* is **q**. Additional heat flux occurs by mechanical dispersion, so the total convective heat flux is

  (27)

The source term describes the rate of heat produced by a chemical reaction, injection, or other means

 S = *Rh* (28)

where *Rh* is the rate of heat energy produced per unit volume. Substituting (26) through (28) into (7) gives the equation for heat transport by convection and conduction

 

Combining terms

  (29)

If *c*p is uniform and constant, then we can simplify to get

  (30)

with the thermal diffusivity as

  (31)

so the thermal dispersion is



and if the thermal diffusivity is uniform

  (32)

where we used . The Laplacian operator is

  (33)

**Example 4: Conservation of Momentum**

Conservation of momentum is expressed by setting , where *v* is velocity, and it follows that *c* is a momentum density. . In a porous medium, , and in a continuous fluid we set *n*=1 to get

  (34)

Momentum flux is , which is the same units as stress.

Momentum can be advected, so applying (3) for a continuous fluid

  (35)

The analogy to diffusion is

  (36)

where (L2T2) is the stress on the fluid.

The rate of production of momentum internally is regarded to be a result of body forces . An example of a body force is **F** = g  where is the unit weight, which can be regarded as a force per volume or a pressure per unit length. The unit weight is the pressure exerted by a fluid per unit depth.

Substituting into (7)

  (37)

Rearranging slightly

  (38)

The fluid density changes only slightly in most flows involving liquids. In these cases, the fluid is commonly assumed to be incompressible, so *d*/*d*t = 0, and we can divide through by  to get

  (39)

*Momentum balance in a Newtonian fluid—the Navier-Stokes Equation*

The momentum balance (39) can be tailored to different materials by describing how stresses occur in that material. To do this for a fluid, we start with describing the fluid velocity

  (40)

where **i**x is a unit vector. Shear stress in a linearly viscous fluid is proportional to the gradient in velocity perpendicular to the flow, so

  (41)

where  (mu) is the dynamic viscosity. This concept can be expanded to include normal stresses due to pressure, so the stresses in a Newtonian fluid are

  (42)

This can be written in a more compact way using index notation

  (43)

where the indices *i* and *j* are coordinate directions, *x,y,z*, and here *u* is the velocity in the direction of the index, *x* is the coordinate direction in the direction of the index. The term ij is kronicker delta, which is equal to 1 when *i = j*, but otherwise it is equal to zero.

The minus sign in front of the pressure is because the typical sign convention is for compressive stress to be negative and tensile stress to be positive. Applying the nabla operator to (43), or taking the divergence of the stress tensor, results in

  (44)

where the last term is the Laplacian of the velocity vector, which is

  (45)

Substituting (44) into (39) gives the Navier-Stokes equation for a linearly viscous fluid

  (46)

The terms in the Navier-Stokes equation represent the following processes



The Navier-Stokes equation is the basis for simulations of fluid flow.

*Momentum Conservation in an elastic solid—Navier equation*

Deformation in an elastic solid is described by the displacement vector

 

where the *d* subscript is used to distinguish displacement from velocity, which is expressed as *u, v, w* above. Stresses are related to strain in an elastic solid by Hooke’s Law as

  (47)

which can be written in a more compact form using index notation

  (48)

where *G* is the shear modulus and  is Lame’s constant.

Strains are defined as displacement gradients, so the normal strains are

  (49)

and shear strains are

  (50)

The volumetric strain is

  (51)

Recall that *u, v, w* are used to indicate the velocities in the *x, y, z* directions. The subscript *d* is used above to distinguish displacement from the velocity. These two quantities are closely related, however.

  (52)

or

  (53)

Substituting (47) into the momentum equation (38) is

  (54)

where the term because the displacements are small. The term on the right side is used to analyze rapid changes, like seismic waves. For quasi-static problems, the term on the right side is zero, so

  (55)

It is convenient to express this equation in terms of displacements. To see how consider expanding (55)

  (56)

Another way to write this is

  (57)

The expression above uses a convention that says you increment and sum the repeated subscript in the derivative operator. In this case, the repeated subscript is *j*, so you increment *j* through *x, y, z* while holding *i* constant, and then sum the three resulting terms. This would give you one of the previous equations. Changing *i* and repeating the process will give the other two equations.

Using (48) and substituting into (56)

 

Grouping terms and expanding each equation in (50)

 

 

 

Substituting in the definition of strain in terms of displacements in (49) and (50)

simplifying the right side in several steps

 

 

 

 

Substituting back into (56) and repeating for the other two equations gives

  (58)

 

 

The three equations above can be written using subscript notation as

  (59)

where each equation is represented by a different value of *i*, and the repeated subscript *j* in the deriviative means to increment through x, y, z and sum the three resulting terms.

The Navier equation (58 or 59) is used to simulate deformation of an elastic solid.