Using Machine Learning for Computational Fluid Dynamics

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May 2019

1 Introduction

This experiment introduces a more efficient way to compute fluid diffusion. The fluid in this scenario is heat. The case at hand references a cube that has heat applied on one side. The temperature at all sides is known, but the internal temperature is not. There is a numerical method for determining the temperature inside the cube. This is done by using finite difference formulations. Here, and throughout this paper, temperature is represented as the variable [u] and heat flow by the variable [q].

$$\Delta u(x, y, z) = 0 \tag{1}$$

$$\frac{\partial^2 u(x,y,z)}{\partial x^2} + \frac{\partial^2 u(x,y,z)}{\partial y^2} + \frac{\partial^2 u(x,y,z)}{\partial z^2} = 0 \tag{2}$$

This heat approximation procedure is completed with respect to grid points that are spaced evenly within the cube. After interpolating all of the grid points, an approximate solution is found for computing internal temperature. This Finite Difference Formulations method is limited due to having a solution only along the grid. The machine learning algorithm has excelled over traditional methods by providing a solution at any point. The machine learning technique used for this problem was **supervised learning**. Supervised learning depends on given data to build an optimized solution. The given data are the inputs and the outputs; based on this data the solution is created. This data "trains" the model. Training is a procedure within supervised learning where the model learns from the data given. The term "learn" is based off of applying weights (values) to the formula being created. First, the formula with current weights has an input given that is the same as an input and output pair. The output of the model is then measured against the output known. The output of the model being optimized is efficient only if the weights are updated correctly. Here the partial derivative come in to measure how much the weights need to be changed. At each neuron, where the equation exists, the partial derivative (with respect to the weights) is taken.

2 Background

The equations given in the introduction (equation [1] and [2]) comes from the first law of thermodynamics and equations from heat flow with u representing temperature.

$$\dot{E}_{in} + \dot{E}_g - \dot{E}_{out} = \dot{E}_s \tag{3}$$

This law states that the energy of a system is constant. The scenario that is being dealt with in this experiment considers that no heat is being generated or stored. The third equation shows heat flow with respect to x. It should be known that the **energy in** and the **energy out** analysis includes all 3 dimensions in this experiment; but for simplicity, the heat flow equation below for energy in and out of the system only includes x.

$$\begin{cases} \dot{E}_g = \dot{q}dxdydz = 0 \\ \dot{E}_s = \rho C_p \frac{\partial T}{\partial t} dxdydz = 0 \\ \dot{E}_{in} = \dot{q}_x \\ \dot{E}_{out} = \dot{q}_{x+dx} \end{cases}$$

It can be seen that all that is left is the analysis of the rate of energy in minus the rate of energy out, with the sum of these equal to zero. The equations [4] and [5] show the fundamental conditions for this experiment.

$$\dot{E}_{in} - \dot{E}_{out} = 0 \tag{4}$$

$$\dot{q}_x - \dot{q}_{x+dx} = 0 \tag{5}$$

3 Conservation of Energy to Laplacian Equation

The fundamental equations above are described the by the energy conservation law. The first law is being applied to a cube, which is our system. What each aspect of this conservation of energy represent is analyzing the heat flow with respect to a cube. This cube is represented by coordinates in the x, y, and z. When analyzing the heat flow within this cube, it is seen that the importance is placed on the x, y, and z direction but also some distance [dx] away from x, y, and z since we are analyzing the whole space. When analyzing each direction with respect to an initial point within the cube, the other two coordinates are held constant while analyzing temperature change with respect to the third dimension that is changing [dx].

The Energy out of the equation is represented as heat flow with respect to a coordinate **'x'** plus some constant **'dx'** distance away using Taylor series. This constant distance is the same throughout every coordinate. The first equation below represents the energy conservation law and the second equation is the Taylor Series expansion equation. Taylor series is used for approximating some function as the distance changes a very small amount. It uses a known value at a current point to find out the value at some (dx) distance away from current x. Since the temperature is known at the borders of this experiment this makes Taylor series an efficient method for a numerical solution. The equation below is Taylor Series written to the first order partial derivative and the function that is being approximated is heat flow. The end equation is written in terms of temperature. Next will be discussed how this is changed using Fourier's Law.

$$\dot{q}_{x+dx} = \dot{q}_x + \frac{\partial q}{\partial x}\Delta x \tag{6}$$

It can be seen that the equation above can be substituted into the original [5th] equation. The result and transformation is below.

$$\dot{q}_x - [\dot{q}_x + \frac{\partial q}{\partial x}\Delta x] = 0 \tag{7}$$

$$\frac{\partial q}{\partial x}\Delta x = 0 \tag{8}$$

$$\frac{\partial q}{\partial x} = 0 \tag{9}$$

Considering that the end **Laplacian** equation [1 and 2] is a representation of temperature and the initial energy conservation equation is in terms of heat flow, we look at the steps that got us there and the concepts behind it. The rate of energy going in and out of our system is represented as heat flow which is **q dot**.

$$\dot{q} = -kA\frac{\partial u}{\partial x}$$

The combination of Fourier's law and equation [9] is below.

$$\dot{q}_x - [\dot{q}_x + \frac{[\partial](-kA)\partial u}{[\partial x]\partial x}\Delta x] = 0 \tag{10}$$

$$\frac{\partial^2 u}{\partial x^2} = 0 \tag{11}$$

This result depends on k which is the thermal conductivity and is held constant as well as A which is area. Fourier's law explains how the energy conservation equation is represented as heat flow but gets transformed to change in temperature. So for every instance where **q dot** appears in the conservation of energy equation, we use Fourier's law to represent temperature since this is what we are approximating.

4 Taylor Series for a Numerical Solution

This experiment relied on using Taylor series expansion for the data provided in the artificial neural network. This method is typical for approximating temperature but the limitations show when wanting an analytic solution. The numerical solution that is provided by this method is accurate, but refers to having a solution for specific values. Although the temperature is known with respect to a certain coordinate, there are unknowns within these points. From the transformation of Energy Conservation to Fourier's Law, we get the equation due to this relationship. We use the Taylor series expansion formula to get the final equation. When the solution from equation [12] is used for every axis [x,y,z] then we get the equation below.

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0 \tag{12}$$

This is the Laplacian equation. Taylor series is used to get the numerical solution using this equation. The equation below represents the relationship between these two equations.

$$\frac{u_{x+dx} + u_{x-dx} + u_{y+dy} + u_{y-dy} + u_{z+dz} + u_{z-dz} - 6u}{\Delta x^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \tag{13}$$

$$\Delta x = \Delta y = \Delta z \tag{14}$$

The numerator can only be Δx^2 because of the conditions in equation 14. The ultimate goal is to have numerical values for the temperature as a function of x,y, and z. With the above equation from Taylor Series it is possible to isolate u. Below is the result which then gives us the final numerical solution for computing internal temperature.

$$u_{ijk} = \frac{u_{x+dx} + u_{x-dx} + u_{y+dy} + u_{y-dy} + u_{z+dz} + u_{z-dz}}{6} \tag{15}$$

5 The Artificial Neural Network

The inputs in the neural network model are coordinate values. The output of the model is temperature values. A model is built with in the computer program using R programming language. In order for the model to be optimized, it has to be trained. The training of our model is done with the values gathered from the Taylor series formulations from equation [15]. The model is built based on the given data (inputs and outputs). The training takes place using a procedure called back-propagation. Once a coordinate value is an input the output the model produced is measured against the values from Taylor Series. This can only be done along the coordinates, but is efficient enough to build the weights for the model. This is done iteratively until the model's output is significantly close to the actual output.

6 References

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