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Numerical Resolution of Fluid Dynamic Problems using a Saddle Point Variational Formulation

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Variational methods are useful for finding numerical solutions of differential equations, which are the corresponding Euler-Lagrange equations to the stationary condition of the functional. Usually the functional is a maximum or a minimum with respect to some function, but in some cases the functional is a saddle point. In this work a saddle point variational formulation is proposed to solve fluid dynamic problems, and the saddle point is found through an iterative method using the optimization software GAMS. Two case studies are solved to show the applicability of the proposed method, one for a single fluid in a two dimensional laminar flow in a pipe and another for a one dimensional turbulent flow for gas-liquid column.
Key Words: variational formulation, saddle point, fluid dynamics.

1. Introduction

Fluid dynamic problems are usually solved as a set of partial differential equations, given by the momentum balance and the continuity equation (Bird et al, 2002). There are many methods available, ranging from analytical solutions for simple problems to numerical methods for more complicated ones, and the finite volume methods is one with widespread use.

Variational methods have been used only on a limited number of cases in fluid dynamic problems, mostly due to the lack of a corresponding variational formulation where the stationary condition corresponds to the original set of differential equations.

In general, variational methods are useful for finding numerical solutions of differential equations, which are the corresponding Euler-Lagrange equations to the stationary condition of the functional. Usually the functional is a maximum or a minimum with respect to some function, but in some cases the functional is a saddle point. In this work a saddle point variational formulation is proposed to solve fluid dynamic problems, and the saddle point is found through an iterative method using the optimization software GAMS. Two case studies are solved, one for a two dimensional laminar flow of a single fluid in a pipe and another for a one dimensional turbulent laminar flow in a gas-liquid column. The results of the first case are compared with an analytical solution, while the second case is compared with the finite volume method.

2. Methodology

2.1 Variational Formulation

The proposed method is described as follows. Consider a function given by:

$$\begin{gathered}\phi(x_1, x_2) = x_1 \cdot x_2 \\ \boldsymbol{x} \in X\end{gathered} \tag{1}$$

This function has a saddle point at $x_1 = 0$ and $x_2 = 0$. While there are many algorithms to find a minimum point, there are not many algorithms for finding a saddle point. Considering a transformation given by:

$$x_1 = \frac{1}{2} \cdot (y_1 + y_2) \tag{2}$$

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$$x_2 = \frac{1}{2} \cdot (y_1 - y_2) \tag{3}$$

then this problem can be rewritten as:

$$\varphi(y_1, y_2) = \frac{1}{4} \cdot (y_1^2 - y_2^2) \\ \boldsymbol{x} \in X \tag{4}$$

Using an iterative procedure, fixing the value of y_2, then the stationary value of y_1 can be found my minimizing the function given by Eq. (4). By a similar procedure, the stationary value of y_2 can be found.

Consider now a functional, given by:

$$I = \iint [\alpha \cdot f(u, v, u_x, v_x) + \beta \cdot g(u, v, u_x, v_x)] \cdot dx_1 \cdot dx_2 \tag{5}$$

s.t.

$$\frac{\partial \alpha}{\partial x_1} + \frac{\partial \beta}{\partial x_2} = 0 \tag{6}$$

$$\frac{\partial u}{\partial x_1} + \frac{\partial v}{\partial x_2} = 0 \tag{7}$$

This functional has stationary conditions given by:

$$f(u, v, u_x, v_x) + \frac{\partial \lambda}{\partial x_1} = 0 \tag{8}$$

$$g(u, v, u_x, v_x) + \frac{\partial \lambda}{\partial x_2} = 0 \tag{9}$$

$$\alpha \cdot \left[\frac{\partial f}{\partial u} - \frac{\partial}{\partial x_1}\left(\frac{\partial f}{\partial u_{x_1}}\right) - \frac{\partial}{\partial x_2}\left(\frac{\partial f}{\partial u_{x_2}}\right)\right] + \beta \cdot \left[\frac{\partial g}{\partial u} - \frac{\partial}{\partial x_1}\left(\frac{\partial g}{\partial u_{x_1}}\right) - \frac{\partial}{\partial x_2}\left(\frac{\partial g}{\partial u_{x_2}}\right)\right] + \frac{\partial \xi}{\partial x_1} = 0 \tag{10}$$

$$\alpha \cdot \left[\frac{\partial f}{\partial v} - \frac{\partial}{\partial x_1}\left(\frac{\partial f}{\partial v_{x_1}}\right) - \frac{\partial}{\partial x_2}\left(\frac{\partial f}{\partial v_{x_2}}\right)\right] + \beta \cdot \left[\frac{\partial g}{\partial v} - \frac{\partial}{\partial x_1}\left(\frac{\partial g}{\partial v_{x_1}}\right) - \frac{\partial}{\partial x_2}\left(\frac{\partial g}{\partial v_{x_2}}\right)\right] + \frac{\partial \xi}{\partial x_2} = 0 \tag{11}$$

Also, consider that the boundary conditions for this problem are chosen so that the set of equations (8)–(11) has the solution $\alpha(x_1, x_2) = 0$ and $\beta(x_1, x_2) = 0$, while $u(x_1, x_2)$ and $v(x_1, x_2)$ have nontrivial solutions.

Now, consider the following change of variables:

$$\alpha = \frac{1}{2} \cdot (u_1 - u_2) \tag{12}$$

$$\beta = \frac{1}{2} \cdot (v_1 - v_2) \tag{13}$$

$$u = \frac{1}{2} \cdot (u_1 + u_2) \tag{14}$$

$$v = \frac{1}{2} \cdot (v_1 + v_2) \tag{15}$$

Using Equations (6) and (7), it is possible to show that:

$$\frac{\partial u_1}{\partial x_1} + \frac{\partial v_1}{\partial x_2} = 0 \tag{16}$$

$$\frac{\partial u_2}{\partial x_1} + \frac{\partial v_2}{\partial x_2} = 0 \tag{17}$$

The functional given by Eq. (5) has a saddle point and it is known that in the stationary condition $\alpha(x_1, x_2) = 0$ and $\beta(x_1, x_2) = 0$. By applying Equations (12)–(15) in Equation (5):

$$I = \frac{1}{2} \cdot \iint \Big[(u_1 - u_2) \cdot f\left(\frac{1}{2} \cdot (u_1 + u_2), \frac{1}{2} \cdot (v_1 + v_2), \frac{1}{2} \cdot (u_1 + u_2)_x, \frac{1}{2} \cdot (v_1 + v_2)_x\right)$$
$$+ (v_1 - v_2) \cdot g\left(\frac{1}{2} \cdot (u_1 + u_2), \frac{1}{2} \cdot (v_1 + v_2), \frac{1}{2} \cdot (u_1 + u_2)_x, \frac{1}{2} \cdot (v_1 + v_2)_x\right)\Big] \cdot dx_1 \cdot dx_2 \tag{18}$$

then an iterative procedure can be used to find the stationary condition of the saddle point:

- set the values of u_2 and v_2 at an initial given profile $u_2^{(0)}$ and $v_2^{(0)}$;
- keep $u_2^{(n)}$ and $v_2^{(n)}$ fixed, then minimize the functional in Equation (18) with respect to u_1 and v_1, satisfying the restriction given by Equation (16), to get $u_1^{(n)}$ and $v_1^{(n)}$;
- make $u_2^{(n+1)} = u_1^{(n)}$ and $v_2^{(n+1)} = v_1^{(n)}$;
- repeat until $\left|u_1^{(n+1)} - u_1^{(n)}\right| \le \varepsilon$ and $\left|v_1^{(n+1)} - v_1^{(n)}\right| \le \varepsilon$.

In this iterative procedure, the values of u_2 and v_2 are updated using the knowledge that in the stationary point $\alpha = 0$ and $\beta = 0$, which implies that $u_2 = u_1$ and $v_2 = v_1$. In order to have good convergence, a relaxation factor ω can be used as follow:

$$u_2^{(n+1)} = (1 - \omega) \cdot u_2^{(n)} + \omega \cdot u_1^{(n)} \tag{19}$$

$$v_2^{(n+1)} = (1 - \omega) \cdot v_2^{(n)} + \omega \cdot v_1^{(n)} \tag{20}$$

Finding the stationary value of Equation (18), satisfying restrictions (16) and (17), is equivalent to solving the set of differential equations given by (7)–(9).

2.2 Mathematical Model

General mass and momentum balance equations for single fluids can be found in Bird et al (2002), while for two phases flow can be found in Torvik and Svendsen (1990), and Grienberger and Hofmann (1992).
The fluid dynamic model considers a general heterogeneous system with two phases, which could be gas-solid, liquid-solid, gas-liquid, or liquid-liquid (immiscible). These two phases here are designated by $i = 1{,}2$. The equations for the steady state isothermal two phase flow in cylindrical coordinates with axi-symmetry (*r*, *z*) are given by:

- Volumetric fraction balance:

$$\varepsilon_1 + \varepsilon_2 = 1 \tag{21}$$

- Mass balance for $i = 1{,}2$:

$$\frac{1}{r} \cdot \frac{\partial}{\partial r}\left[r \cdot \rho_i \cdot \varepsilon_i \cdot v_{ir} - r \cdot D_{ij} \cdot \frac{\partial}{\partial r}(\rho_i \cdot \varepsilon_i)\right] + \frac{\partial}{\partial z}\left[\rho_i \cdot \varepsilon_i \cdot v_{iz} - D_{ij} \cdot \frac{\partial}{\partial z}(\rho_i \cdot \varepsilon_i)\right] = \xi_i \tag{22}$$

$$\xi_1 + \xi_2 = 0 \tag{23}$$

If there is no mass transfer between the phases, then $\xi_i = 0$.

- Momentum balance for $i = 1{,}2$:

$$\frac{1}{r}\cdot\frac{\partial}{\partial r}(r\cdot\rho_i\cdot\varepsilon_i\cdot v_{ir}\cdot v_{ir})+\frac{\partial}{\partial z}(\rho_i\cdot\varepsilon_i\cdot v_{iz}\cdot v_{ir})=+\rho_i\cdot\varepsilon_i\cdot g_r+\xi_i\cdot v_{ir}+F_{ijr}+L_{ijr}$$
$$-\varepsilon_i\cdot\frac{\partial p}{\partial r}+\frac{1}{r}\cdot\frac{\partial}{\partial r}\left[r\cdot\mu_i\cdot\varepsilon_i\cdot 2\cdot\frac{\partial v_{ir}}{\partial r}\right]-\mu_i\cdot\varepsilon_i\cdot 2\cdot\frac{v_{ir}}{r^2}+\frac{\partial}{\partial z}\left[\mu_i\cdot\varepsilon_i\cdot\left(\frac{\partial v_{ir}}{\partial z}+\frac{\partial v_{iz}}{\partial r}\right)\right] \tag{24}$$

$$\frac{1}{r}\cdot\frac{\partial}{\partial r}(r\cdot\rho_i\cdot\varepsilon_i\cdot v_{ir}\cdot v_{iz})+\frac{\partial}{\partial z}(\rho_i\cdot\varepsilon_i\cdot v_{iz}\cdot v_{iz})=+\rho_i\cdot\varepsilon_i\cdot g_z+\xi_i\cdot v_{iz}+F_{ijz}+L_{ijz}$$
$$-\varepsilon_i\cdot\frac{\partial p}{\partial z}+\frac{1}{r}\cdot\frac{\partial}{\partial r}\left[r\cdot\mu_i\cdot\varepsilon_i\cdot\left(\frac{\partial v_{ir}}{\partial z}+\frac{\partial v_{iz}}{\partial r}\right)\right]+\frac{\partial}{\partial z}\left[\mu_i\cdot\varepsilon_i\cdot 2\cdot\frac{\partial v_{iz}}{\partial z}\right] \tag{25}$$

For a vertical pipe, $g_z=-g$. For a horizontal pipe, both g_z and g_r may be neglected.
When the flow is in laminar regime, the velocity in the previous equations is the actual velocity, while the viscosity is just the viscosity for a Newtonian fluid, μ. However, when the flow is in turbulent regime, the velocity is an average over time fluctuations, even when the model is for permanent flow, and the viscosity is an effective viscosity given by:

$$\mu^{\text{eff}}=\mu+\mu^{(t)} \tag{26}$$

The turbulent viscosity, $\mu^{(t)}$, can be calculated using different turbulence models, such as $k-\varepsilon$ (Hillmer et al, 1994). In this work, it is considered a zero order turbulence model (Menzel et al, 1990; Chen et al, 1995), for the sake of simplicity, since in this case $\mu^{(t)}$ is a function of local position and not on local velocity profiles. However, in zero order models the turbulent viscosity depends on the wall shear stress.
The diffusivity of one phase into another (D_{ij}) affects the distribution of the volume fractions of the phases inside the reactor volume (ε_i), even if they are immiscible. It can be shown that $D_{ji}=D_{ij}$ and that these values may be variable. It can also be shown that for turbulent flow the Schmidt number is equal to 1, so that:

$$D_{ij}^{(t)}=\frac{\mu_i^{(t)}}{\rho_i}=\frac{\mu_j^{(t)}}{\rho_j} \tag{27}$$

The force between the phases can be described by:

$$F_{ijr}=C_D\cdot\varepsilon_i\cdot\varepsilon_j\cdot(v_{jr}-v_{ir}) \tag{28}$$

$$F_{ijz}=C_D\cdot\varepsilon_i\cdot\varepsilon_j\cdot(v_{jz}-v_{iz}) \tag{29}$$

where it can be seen that $F_{jir}=-F_{ijr}$ and $F_{jiz}=-F_{ijz}$. The value of C_D may be considered either a constant or a function of radial position only, and it can have different values for different systems.
The transversal lift force is also known as the Magnus force. Here it is considered in the most general case, where both phases can affect each other. In the case considered in this work, where the velocities have only components on r and z directions, it results in:

$$L_{ijr}=+0.5\cdot C_L\cdot\varepsilon_i\cdot\varepsilon_j\cdot(v_{iz}-v_{jz})\cdot\left[\rho_i\cdot\left(\frac{\partial v_{ir}}{\partial z}-\frac{\partial v_{iz}}{\partial r}\right)+\rho_j\cdot\left(\frac{\partial v_{jr}}{\partial z}-\frac{\partial v_{jz}}{\partial r}\right)\right] \tag{30}$$

$$L_{ijz}=-0.5\cdot C_L\cdot\varepsilon_i\cdot\varepsilon_j\cdot(v_{ir}-v_{jr})\cdot\left[\rho_i\cdot\left(\frac{\partial v_{ir}}{\partial z}-\frac{\partial v_{iz}}{\partial r}\right)+\rho_j\cdot\left(\frac{\partial v_{jr}}{\partial z}-\frac{\partial v_{jz}}{\partial r}\right)\right] \tag{31}$$

The boundary conditions for this model are the usual ones, both for the velocities at the inlet, and for the centre and the walls.

2.3 Numerical Implementation

The proposed method was implemented in GAMS, solved with the CONOPT3 solver. For a single-phase fluid, Equation (18) is used, while for two phases fluid flows a more general functional is used that results in the model described in Section 2.2. The derivatives were calculated using second order finite differences, while the integrals were calculated using the trapezoidal rule, which for cylindrical coordinates is given by:

$$\int_{x_i}^{x_{i+1}} y\cdot x\cdot dx=\frac{\Delta x}{6}\cdot[y_i\cdot(2\cdot x_i+x_{i+1})+y_{i+1}\cdot(x_i+2\cdot x_{i+1})] \tag{32}$$

3. Results and discussion

Two case studies were solved using the proposed method. The first case considers a two-dimensional laminar flow of a single fluid in a pipe and the results were compared with an analytical solution. The second case considers a one-dimensional turbulent laminar flow in a gas-liquid column and the results were compared with a numerical solution using the finite volume method.

3.1 Two dimensional laminar flow for a single fluid

The laminar flow of a single fluid in a pipe was calculated using the proposed method. The equations were written in a dimensionless form, so that only two parameters were required to characterize the flow, the Reynolds number and the relation of length to radius of the pipe (L/R). Table 1 shows the results for the axial velocity, using 50 intervals in the radial direction and 20 intervals in the axial direction, for different radial and axial positions. In order to have good convergence, a relaxation factor $\omega = 0.05$ was used. A very low Reynolds number was used, so that a fully developed flow was achieved with a short pipe length. The results were compared with an analytical solution presented by Guirardello (2015), with good results. Also, the parabolic profile at a fully developed flow was achieved, with differences between analytical and numerical solutions due to the size of the interval used in the radial direction.

Table 1. Axial velocity v_z/v_0 for Re=2 and L/R=4

r/R	z/L=0.00	z/L=0.05	z/L=0.10	z/L=0.25	z/L=0.50	z/L=1.00
0.00	1.000000	1.126244	1.401038	1.927852	2.000300	2.000106
0.10	1.000000	1.126709	1.400182	1.911969	1.980294	1.980112
0.20	1.000000	1.128069	1.397136	1.863589	1.920278	1.920127
0.30	1.000000	1.130163	1.390264	1.780616	1.820252	1.820150
0.40	1.000000	1.132552	1.376165	1.659878	1.680220	1.680175
0.50	1.000000	1.134087	1.348304	1.497709	1.500186	1.500192
0.60	1.000000	1.131739	1.294143	1.290831	1.280150	1.280180
0.70	1.000000	1.117222	1.189069	1.037201	1.020104	1.020118
0.80	1.000000	1.065997	0.983477	0.735303	0.719987	0.720019
0.90	1.000000	0.893763	0.576895	0.382547	0.380284	0.380148
1.00	1.000000	0.000000	0.000000	0.000000	0.000000	0.000000

3.2 One dimensional turbulent flow for two fluids

The turbulent flow of a gas-liquid bubble column was calculated with the proposed method. The liquid and the gas phases are fed at the bottom of a vertical column. Since only a one-dimensional model was solved, in the radial direction, the length of the column was considered to be long enough for a fully developed flow.

The column considered had a radius of 30 cm. The liquid mass flow was $400\ \mathrm{g/s}$, with density $\rho_l = 0.70\ \mathrm{g/cm^3}$ and viscosity $\mu_l = 0.0090\ \mathrm{g.cm^{-1}.s^{-1}}$. The gas mass flow was $10\ \mathrm{g/s}$, with density $\rho_g = 0.0012\ \mathrm{g/cm^3}$ and viscosity $\mu_g = 0.0002\ \mathrm{g.cm^{-1}.s^{-1}}$. The turbulent viscosity and mass diffusivity were calculated using a correlation proposed by Chen et al (1995) and Menzel et al (1990), with $k_L = 0.1$ and $P'_w/\rho_m = 1000\ \mathrm{cm^2/s^2}$, considering an homogeneous flow for the gas bubbles. The drag force between phases was calculated using $C_D = 50\ \mathrm{g.cm^{-3}.s^{-1}}$. The Magnus force was calculated considering $C_L = -1$.

This case study was solved with the variational method, using 20 intervals in the radial direction and a relaxation factor $\omega = 0.50$ for convergence, using GAMS and CONOPT3. It was also solved with the finite volume method, using 20 intervals in the radial direction, using EXCEL.

Nonlinear optimization problems usually are sensitive to initial estimates in some variables, so in order to compare the two methods, the liquid and gas hold-ups in the variational method were fixed using the same values of hold-ups found in the finite volume method.

Results are presented in Table 2, where the 2nd through 6th columns refer to the numerical solution using the finite volume method, while the 7th and 8th columns refer to the numerical solution using the variational method. The recirculation pattern for the liquid phase is easily visible, were the liquid axial velocity is negative next to the column wall, indicating a descendent flow, and positive in the middle of the column. This recirculation pattern in the liquid phase is a phenomenon that is observed experimentally in two phases flow (Chen et al, 1995; Menzel et al, 1990).

Table 2: Comparison between finite volume and variational methods (all units in CGS).

r	$v_{z,l}$	$v_{z,g}$	$v_{r,l}$	$v_{r,g}$	ε_l	$v_{z,l}$	$v_{z,g}$
0.0	2.207	15.957	0.00000	0.00000	0.7783	2.427	16.177
1.5	2.185	15.935	0.00018	-0.00062	0.7783	2.401	16.150
3.0	2.120	15.869	0.00035	-0.00122	0.7783	2.320	16.068
4.5	2.013	15.762	0.00050	-0.00175	0.7783	2.200	15.948
6.0	1.872	15.620	0.00063	-0.00220	0.7784	2.048	15.795
7.5	1.703	15.450	0.00073	-0.00255	0.7784	1.868	15.615
9.0	1.512	15.258	0.00080	-0.00280	0.7785	1.667	15.413
10.5	1.308	15.053	0.00084	-0.00296	0.7785	1.452	15.197
12.0	1.095	14.839	0.00086	-0.00302	0.7786	1.228	14.971
13.5	0.881	14.625	0.00085	-0.00300	0.7787	1.000	14.743
15.0	0.671	14.413	0.00083	-0.00292	0.7787	0.775	14.517
16.5	0.469	14.210	0.00079	-0.00278	0.7788	0.556	14.297
18.0	0.278	14.019	0.00074	-0.00260	0.7788	0.346	14.086
19.5	0.103	13.842	0.00067	-0.00236	0.7789	0.149	13.888
21.0	-0.055	13.683	0.00059	-0.00208	0.7789	-0.034	13.704
22.5	-0.191	13.546	0.00049	-0.00174	0.7789	-0.200	13.538
24.0	-0.301	13.436	0.00037	-0.00130	0.7790	-0.345	13.392
25.5	-0.376	13.361	0.00020	-0.00069	0.7790	-0.466	13.271
27.0	-0.400	13.336	-0.00009	0.00033	0.7790	-0.558	13.179
28.5	-0.332	13.407	-0.00079	0.00278	0.7789	-0.613	13.136
30.0	0.000	0.000	0.00000	0.00000	0.7788	0.000	0.000

4. Conclusions

The proposed method showed very good results, being able to give reliable and accurate results for two case studies, having good agreement with other methods.

One interesting feature of the variational method is that the pressure field does not need to be explicitly calculated, since it is the Lagrangian multiplier associated with the continuity equation. The pressure can be found later, after the velocity profiles are calculated, using GAMS and calling for the marginal value of that restriction after a ‘solve’. In this work all physical properties were considered constant, but for a problem where physical properties change with pressure this variation can be easily computed after each loop of the iterative procedure.

The numerical application of the variational method still needs some improvement, due to some numerical difficulties, related to terms with different orders of magnitude and with initial estimates in the optimization.

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