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FINITE DIFFERENCE METHOD FOR FLUIDS DYNAMICS Applications in Python and C++





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PREFACE

The accessibility of computers has resulted in a novel era of teaching and learning, expanding traditional science and engineering curricula to include scientific computing is both desired and required. Numerical simulation is a cost-effective alternative to actual experimentation due to its portability and minimal overhead. The new framework has prompted the creation of texts written from a modern perspective, with mathematics and computer programming features integrated into the discourse. This modern directive theory and execution are complementary and provided in a sequential order. A different approach involves connecting computational approaches and simulation algorithms, as well as turning equations into computer code instructions directly after problem formulation. The seamless integration of scientific computer tools into traditional discourse provides a great forum for improving analytical abilities and gaining physical knowledge.

The goal of this book is to provide the reader with all of the tools needed to understand the topics of computational fluid dynamics, beginning with brief references to fluid mechanics, demonstrating the difficulties in solving the governing equations, and progressing to the various numerical approaches used in the scientific literature, with a focus on the finite difference method.

Furthermore, the problem of turbulence and vortex dynamics was highlighted, examining the turbulence models and the DNS method. Finally, we wanted to present some engineering applicaIV Preface

tions that make use of different numerical methodologies.

The presentation of the material is distinguished by the practical component of the text to make the exposition of the concepts clearer, so certain paragraphs feature examples of numerical code generated in a Python environment with some C++ applications.

> Rome, October 2024 Biagio Saya

Part I

FUNDAMENTAL CONCEPT

1

INTRODUCTION

1.1 THE NATURE OF FLUIDS

There are several possibilities to watch fluids flowing in our everyday environment, such as smoke from a chimney, water in a river or waterfall, or the buffeting of a strong wind. Fluid flow occurs in response to external conditions, such as boundary motion, surface force, or body force. The evolution of a transient flow and the structure of a steady flow established after an initial start-up period are governed by two fundamental principles of thermodynamics and classical mechanics: mass conservation, and Newton's second law for the motion of a fluid. For fluid flows, be they laminar or turbulent, the governing laws are embodied in the Navier–Stokes equations, which have been known for over a century.

1.2 COMPUTATIONAL PHYSICS

As previously introduced, humans have long been fascinated with fluid behavior. However, contrary to common opinion, these events exhibit complex characteristics that are impossible to predict using a simple linear equation. It is generally accepted that the Naiver-Stokes equations (NS) can explain fluid motion. The intricacy of fluid motion necessitates the employment of numerical techniques, resulting in the term "*Computational Physics*". This field has seen a surge of development in the previous thirty years, both theoretically and practically. Improvements in numerical approaches, along with rapid advancements in computer technology, have resulted in many formerly intractable fluid dynamics problems being routinely solved. The primary aim of this discipline of science is to solve partial derivative equations using a numerical model that produces an approximate solution. The numerical solution's congruence with real-world experience and experimental observation warrants further investigation.

Considering the diversity and complexity of fluid flows, it is quite remarkable that the relatively simple Navier–Stokes equations describe them accurately and in complete detail, and as a consequence (in general) the direct approach to solving the Navier–Stokes equations is impossible. So, while the Navier–Stokes equations accurately describe turbulent flows, they do not provide a tractable model for them. For this reason, the direct approach to solving the Navier–Stokes equations for turbulent flows, also called direct numerical simulation (DNS), becomes a workable solution. This method becomes fundamental for the study of flow in the high-Reynolds-number and it is nevertheless a powerful research tool for investigating the turbulent flow through statistical models that can be used to calculate the properties of turbulence.

2.1 OVERVIEW

Everyday life provides us with an intuitive understanding of fluid motion: the smoke from a cigarette or a fire. Despite this, it is easy to see how, in most circumstances, we are presented with examples of chaotic phenomena, making the topic's discussion challenging. The non-regularity of fluids can be summarized in the turbulent regime proposed by Reynold.

More specifically Turbulence is also mentioned to describe the flow of a stream in a river, with important consequences concerning the sediment transport and the motion of the bed. The rapid flow of any fluid passing an obstacle or an airfoil creates turbulence in the boundary layers and develops a turbulent wake which will generally increase the drag exerted by the flow on the obstacle (and measured by the well known C_D coefficient): in this perspective, turbulence has to be avoided in order to obtain better aerodynamic performance for cars or planes. The majority of atmospheric or oceanic currents cannot be predicted accurately and fall into the category of turbulent flows, even on large planetary scales. Small-scale turbulence in the atmosphere represent an obstacle to the accuracy of astronomic observations, and observatory locations have to be chosen in consequence. The atmospheres of planets such as Jupiter (figure 1) and Saturn, the solar atmosphere or the Earth's outer core are turbulent. Galaxies look strikingly like the eddies which are observed in turbulent flows such as the mixing layer between two flows of different velocities and are, in a manner of speaking, the eddies of a turbulent universe. Turbulence is also produced in the Earth's outer

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magnetosphere, due to the development of instabilities caused by the interaction of the solar wind with the magnetosphere. Numerous other examples of turbulent flows arise in aeronautics, hydraulics, nuclear and chemical engineering, oceanography, meteorology, astrophysics, and internal geophysics ([Lesieur(2008)]).

In conclusion, the fluids in a turbulent regime exhibit abstruse behavior. As a result, the goal we will pursue will be to investigate turbulence and vortex dynamics, as these are the challenges of the new millennium.



Figure 1: Eddies in Jumpiter observed by JunoCam imager on NASA's Juno spacecraft in December 2018 ([Nasa(2018)])

2.2 INTRODUCTION TO MOTION EQUATIONS

The necessity to study the spectacular behavior of fluid and eddies motion led to conceive an elegant formulation made by equations of Motion, Mass and energy balance. This concept can be expressed in a simple formulation suggested from the study of General Relativity that assumes the following formalism ([Landau and Lifshitz(2013)]),

$$\partial T_i^k / \partial x_k = 0 \tag{2.1}$$

 T_i^k represents the stress tensor energy and $\partial/\partial x_k$ express the partial derivative in 4-space, which are the three Cartesian coordinates and the time. But omitting the relativistic approach in classic formalism the equations of motion for a general Newtonian fluid will now be established. In doing so the fluid will be considered to be a continuum. In a continuum, the smallest volume element considered dV is still homogeneous, i.e. the dimensions of dV are still very large compared to the average distance between the molecules in the fluid. In three–dimensional motion the flow field is given by the velocity vector

$$\vec{v} = \vec{e}_x u + \vec{e}_y v + \vec{e}_z w \tag{2.2}$$

with the three components u, v, w in a Cartesian coordinate system with unit vectors $\vec{e}_x, \vec{e}_y, \vec{e}_z$ and also by the pressure p and the temperature T. To determine these five quantities, there are five equations available: continuity equation, three momentum equations and energy balance ([Schlichting and Kestin(1961)]).

2.3 THE CONTINUITY EQUATION

The classical Newtonian physics assumes conservation of mass m, which can be written as dm/dt = 0. The Balance of mass is a generalization of this equation to the continuum mechanics setting. Consider a tiny differential control volume that can be approximated to the mass flow rate into or out of each of the six surfaces of the control volume and, using Taylor series expansions around the center point, where the velocity components and density are u, v, w, and ρ . For example,

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$$(\rho u)|_{rightside} = \rho u + \frac{\partial(\rho u)}{\partial x} \cdot dx + \frac{1}{2!} \frac{\partial^2(\rho u)}{\partial x^2} \cdot dx^2 + \dots$$
(2.3)

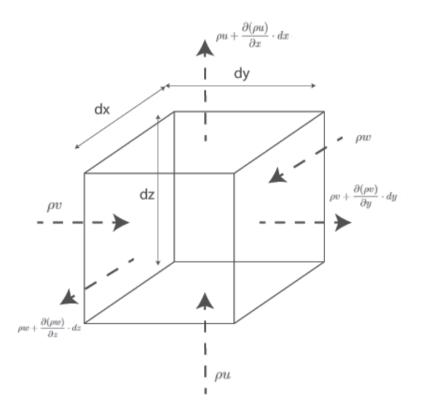


Figure 2: integration domain using

Next, we add up all the mass flow rates through all six faces of the control volume to generate the general (unsteady, incompressible) continuity equation:

$$\sum_{in} \dot{m} = \rho u \, dy \, dz + \rho v \, dx \, dz + \rho w \, dx \, dy \tag{2.4}$$

$$\sum_{out} \dot{m} = \rho u \, dy \, dz + \rho v \, dx \, dz + \rho w \, dx \, dy + \left(\frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial x}\right) \cdot dx \cdot dy \cdot dz$$
(2.5)

where $\sum_{in} \dot{m}$ and $\sum_{out} \dot{m}$ are the net mass flow in and out of the control volume V(t) and neglecting the term higher of second order in Taylor expansion.

The mass m(t) of volume V(t) is expressed in terms of the Eulerian density field $\rho(x, t)$ as

$$m(t) = \int_{V(t)} \rho(x, t) dv$$
 (2.6)

and its derivative, for the Leisbery theorem, becomes

$$\frac{dm}{dt} = \int_{V(t)} \frac{\partial(\rho)}{\partial t} dv \tag{2.7}$$

Using the notion of the density field, the Reynolds transport theorem, and the requirement

$$\int_{V(t)} \frac{\partial(\rho)}{\partial t} dv = \sum_{in} \dot{m} - \sum_{out} \dot{m}$$
(2.8)

with $\nabla \cdot v(x,t)$ the diverge of velocity filed. Then immediately yield the integral form of the balance of mass

$$\int_{V(t)} \left[\frac{\partial \rho}{\partial t} + \rho(x, t) \nabla \cdot \boldsymbol{v}(x, t) \right] dv = 0$$
 (2.9)

where V(t) is an arbitrary volume in the sense that it is the volume obtained by tracking an arbitrarily chosen initial volume $V(t_0)$. Since the volume in the previous equation is arbitrary, and the considered physical quantities are assumed to be sufficiently

smooth, the integral form of the balance of mass leads to the point wise evolution equation

$$\frac{\partial \rho}{\partial t} + \rho(x,t)\nabla \cdot \boldsymbol{v}(x,t) = 0$$
(2.10)

It follows immediately from the continuity equation 2.10 that incompressible flows, i.e. flows of incompressible fluids, are source-free. We have:

$$\frac{\partial \rho}{\partial t} = 0 \qquad \nabla v = 0$$
 (2.11)

2.4 THE MOMENTUM EQUATION

Fluid flow is established in response to an external action mediated by boundary motion, by the application of a surface force, or by the presence of a body force. The evolution of a transient flow and the structure of a steady flow established after an initial start-up period is governed by two fundamental principles of thermodynamics and classical mechanics: mass conservation and Newton's second law for the motion of a fluid parcel. The implementation of Newton's law of motion in continuum mechanics leads to Cauchy's equation of motion, providing us with an expression for the point particle acceleration in terms of stresses, and to the vorticity transport equation governing the point particle rotation. The derivation and interpretation of these equations in general and specific terms, and their solution for simple flow configurations will be discussed.

Newton's second law of motion requires that the rate of change of the linear momentum of a fluid parcel, *M*, is equal to

the sum of the forces exerted on the parcel, including the body force due to gravity \vec{f} and the surface force \vec{P} ,

$$\frac{dM}{dt} = \vec{f} + \vec{P} = \iint_{S(t)} f \cdot ds + \iiint_{V(t)} \rho \cdot g \cdot dV \tag{2.12}$$

where f is the hydrodynamic traction exerted on the parcel surface. Expressing the traction in terms of the stress tensor, we find

$$\frac{dM}{dt} = \iint_{S(t)} \mathbf{n} \cdot \boldsymbol{\sigma} \cdot ds + \iiint_{V(t)} \rho \cdot g \cdot dV \tag{2.13}$$

where the unit normal vector, *n*, points into the parcel exterior. Our next task is to relate the rate of change of the parcel momentum to the fluid density and velocity.

RATE OF CHANGE OF LINEAR MOMENTUM

An expression for the linear momentum arises considering the mass $dm = \rho dv$, and summing the contributions by integration to obtain the rate of change of linear momentum,

$$\frac{d\vec{M}}{dt} = \frac{d}{dt} \int_{\tilde{\rho}(t)} v dm = \iiint_{V(t)} \frac{Dv}{Dt} \rho dV$$
(2.14)

with $\tilde{\rho}$ the density per unit volume (ρdv) and v the fluid velocity.

Note that an equation demonstrated previously expresses the inertial force of the fluid mass. If we want to express the inertial component F_i of a material point with mass m we obtain that $F_i = d/dt(m \cdot v)$.

Substituting the right-hand side of equation 2.14 in the left-hand side of 2.15, we obtain the desired equation of parcel motion,

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$$\iiint_{V(t)} \frac{Du}{Dt} \rho dV = \iint_{S(t)} \mathbf{n} \cdot \boldsymbol{\sigma} \cdot ds + \iiint_{V(t)} \rho \cdot g \cdot dV \quad (2.15)$$

involving the point particle acceleration, the stress tensor, and the body force. Explicitly, the x, y, and z components are,

$$\iiint_{V(t)} \frac{Du}{Dt} \rho dV = \iint_{S(t)} (\sigma_{xx} + \sigma_{yx} + \sigma_{zx}) \cdot ds + \iiint_{V(t)} \rho \cdot g_x \cdot dV$$

$$\iiint_{V(t)} \frac{Dv}{Dt} \rho dv = \iint_{S(t)} (\sigma_{xy} + \sigma_{yy} + \sigma_{zy}) \cdot ds + \iiint_{V(t)} \rho \cdot g_y \cdot dV$$

$$\iiint_{V(t)} \frac{Dw}{Dt} \rho dv = \iint_{S(t)} (\sigma_{xz} + \sigma_{yz} + \sigma_{zz}) \cdot ds + \iiint_{V(t)} \rho \cdot g_z \cdot dV$$

The previous equations are valid irrespective of whether the fluid is compressible or incompressible.

Transforming the surface integral of the traction into a volume integral can be done using once again the Gauss divergence theorem. We obtain

$$\iint_{S(t)} \boldsymbol{n} \cdot \boldsymbol{\sigma} \cdot d\boldsymbol{s} = \iiint_{V(t)} \nabla \cdot \boldsymbol{\sigma} \cdot d\boldsymbol{v}$$
(2.16)

Substituting 2.16 in 2.15, consolidating various terms, and noting that because the volume of integration is arbitrary the combined integrand must vanish, we obtain Cauchy's differential equation governing the motion of an incompressible or compressible fluid,

$$\rho \frac{D\boldsymbol{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{g} \tag{2.17}$$

In index notation,

$$\rho \frac{Du_i}{Dt} = \frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i \tag{2.18}$$

Eulerian Equation

Euler's equation derives from the equation of motion 2.17 by substituting the simplest possible constitutive equation for the stress tensor corresponding to an ideal fluid, Considering the individual components of the volume force to a pressure or spherical stress tensor, we find

$$\nabla \cdot \boldsymbol{\sigma} = -\nabla \cdot \boldsymbol{p} \tag{2.19}$$

The equation of motion then reduces to Euler's equation

$$\rho \frac{Du}{Dt} = -\nabla \cdot p + \rho g \tag{2.20}$$

The associated Eulerian form is

$$\rho\left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla \cdot p + \rho g \tag{2.21}$$

Irrotational flow

Expressing the velocity in terms of the gradient of the velocity potential, ϕ , we find that Euler's equation takes the simple form

$$\rho\left(\frac{\partial\nabla\phi}{\partial t} + \frac{1}{2}\nabla u^2\right) = -\nabla\cdot p + \rho g \qquad (2.22)$$

The acceleration of gravity can be expressed as the gradient of the scalar *s*

$$g = \nabla s = \nabla (g \cdot x) = \nabla (g_x x + g_y y + g_z z)$$
(2.23)

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Substituting this expression in 2.22, assuming that the density is uniform throughout the domain of flow and collecting all terms under the gradient, we find

$$\nabla\left(\frac{\partial\phi}{\partial t} + \frac{1}{2}u^2 + p - \rho gx\right) = 0$$
 (2.24)

Since the spatial derivatives of the scalar quantity enclosed by the parentheses on the left-hand side of 2.24 are zero, the quantity must be independent of position although it may change in time. Euler's equation for rotational flow then reduces to Bernoulli's equation describing the irrotational flow of a uniform-density fluid,

$$\frac{\partial \phi}{\partial t} + \frac{1}{2}u^2 + p - \rho g \mathbf{x} = c(t)$$
(2.25)

where c(t) is an unspecified function of time.

The Navier-Stokes equation

The Navier-Stokes equation follows from the equation of motion 2.17 by substituting the constitutive equation for the stress tensor for a fluid with uniform viscosity, the hydrodynamic volume force.

$$\sigma = -\delta_{ij} \cdot \boldsymbol{p} + \mu \left(\boldsymbol{\epsilon} - \frac{2}{3} \delta_{ij} \operatorname{div} \vec{v}
ight)$$

with δ_{ij} being the unit tensor of Dirac, μ the dynamic viscosity and ϵ the deformation tensor function of the field velocity ([Landau and Lifshitz(2013)]). An explicit form of τ can be expressed as

$$\sigma_{ij} = -p_i + \frac{\mu}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \delta_{ik} \frac{2}{3} \frac{\partial u_k}{\partial x_k} \right)^2$$

Correspondingly, the equation of motion reduces to the Navier-Stokes equation the following form.

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla \cdot \boldsymbol{p} + \mu \nabla^2 \boldsymbol{u} + \rho g \qquad (2.26)$$

There is no analytical solution for Navier-Stokes with the exception of basic examples. In other situations, a numerical or experimental solution must be used. However, it must be taken into account that the great mathematical difficulty of these equations means that only very few solutions are known where the convective terms interact quite generally with the friction terms. However, known particular solutions, such as laminar pipe flow well agree with the experimental results that there is hardly any doubt about the general validity of the Navier–Stokes equations. As a consequence of the Navier–Stokes equations, an equation for the mechanical energy can be derived. If the Navier–Stokes equation in the *x* direction is multiplied by *u*, the one in the *y* direction by *v* and the one in the *z* direction by *w*, and they are summed up, the energy equation for the mechanical energy is found ([Schlichting and Kestin(1961)]).

Following the general protocol of methods based on the vorticity transport equation, we compute the evolution of the flow by advancing the vorticity field using the vorticity transport equation for two-dimensional flow written in the form of an evolution equation for the vorticity. In particular, if we applied the Curl operator at Stokes equation we can obtain the following formulation.

$$\frac{\partial \omega}{\partial t} = -\nabla \times (u\nabla u) + v\nabla^2 \omega \qquad (2.27)$$

where $\nu \equiv \mu / \rho$ is the kinematic viscosity.

$$\frac{\partial \omega}{\partial t} + \omega \nabla \cdot \boldsymbol{u} = -\boldsymbol{u} \nabla \cdot \boldsymbol{\omega} + \nu \nabla^2 \boldsymbol{\omega}$$
(2.28)

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in addiction, in the two dimensional plane *x*, *y* the times $\omega \times \omega = \omega \times \nabla \times u = 0$, so the Vortex Transportation equation becomes (eq. 7.2),

$$\frac{\partial \omega_z}{\partial t} = -\boldsymbol{u} \cdot \nabla \omega_z + \nu \nabla^2 \omega_z \tag{2.29}$$

subject to appropriate derived boundary conditions for the vorticity, while simultaneously obtaining the evolution of the stream function by solving the Poisson equation.

$$\nabla^2 \psi = -\omega \tag{2.30}$$

2.5 ENERGY EQUATION

In order to set up the equation for the energy balance in a flow, we consider a fluid particle of mass $dM = \varrho dV$ and volume $dV = dx \cdot dy \cdot dz$ in a Cartesian coordinate system and follow it on its path in the flow. According to the first law of thermodynamics, the gain in total energy DE_t (the index *t* stands for total energy) in unit time Dt is equal to the heat supplied to the mass element $\dot{Q}Dt$ and the work done on the element \dot{W} Dt. Therefore we have:

$$\frac{DE_t}{Dt} = \dot{Q} + \dot{W} \tag{2.31}$$

Where DE_t/Dt is the energy variation, \dot{Q} the heat flux and \dot{W} the power made by mechanical energy. The \dot{Q} term can be expressed in the following way,

$$\dot{Q} = -dV\,div\,\vec{q} \tag{2.32}$$

where \vec{q} represents a heat flux vector. The total energy E_t generally consists of three parts: the internal energy e, the kinetic

energy $1/2 dM \cdot v^2$ and the potential energy ψ . The following statement holds:

$$dE_t = dV \, \varrho \left(e + \frac{1}{2} \vec{v}^2 + \psi \right) \tag{2.33}$$

Thus the substantial change of the total energy follows as

$$\frac{DE_t}{Dt} = dV \,\varrho \, \frac{D\left(e + \frac{1}{2}\vec{v}^2 + \psi\right)}{Dt} \tag{2.34}$$

The total rate of work done on the mass element of volume dV is:

$$\dot{W} = dV \,\nabla(\sigma \vec{v}) \tag{2.35}$$

if we combine Eq. 2.31, 2.32, 2.33 and 2.34 we can obtain:

$$\varrho \frac{D\left(e + \frac{1}{2}\vec{v}^2 + \psi\right)}{Dt} = -\nabla \vec{q} + \nabla\left(\sigma \,\vec{v}\right)$$
(2.36)

Last we can write the heat flux \vec{q} as

$$\vec{q} = -\lambda \,\nabla T \tag{2.37}$$

T corresponds to the scalar temperature field, λ to the heat conduction coefficient and σ represents the stress tensor.

2.6 DRAG AND LIFT FORCE

It is known that external forces occur when an object is moving into a fluid. These are the drag, lift, and torque force ([Landau and Lifshitz(2013)]). They depend on the velocity U, the density ρ , the relative contact surface S, and a constant number C, which can be called Drag C_D , Lift C_L , or Torque C_{ϕ} Coefficient. These coefficients can be calculated through the total force in *x* or *y* direction, called respectively like F_D and F_L .

$$F_D = \int_{\gamma} p \cdot e_x \, d\gamma + \int_{\gamma} \tau \cdot e_x \, d\gamma \qquad (2.38)$$

$$F_L = \int_{\gamma} p \cdot e_y \, d\gamma + \int_{\gamma} \tau \cdot e_y \, d\gamma \tag{2.39}$$

while the torque force is function of the radius vector \vec{r} and can be expressed as

$$F_{\phi} = \int_{\gamma} \vec{\tau} \cdot \vec{r} \, d\gamma \tag{2.40}$$

 n_x and n_y represent respectively the normal vector in the direction along x and y while γ is the perimeter of immerse boundary which is calculated by the Drag Coefficient. It can be a squared, cylinder, or complex geometry.

The C_D , C_L are expressed in the following equation,

$$C_D = \frac{F_D}{\rho U^2 S_D}$$
$$C_L = \frac{F_L}{\rho U^2 S_L}$$

with S_D and S_L the projection surface of the object along the flow direction or perpendicular to it. From the experimental results, it is known that the C_D varies with Reynolds Number R_e . In the case of a cylinder, it was observed that with a very small Reynolds $R_e << 1$ the drag is proportional to the linear dimension of the body and to the velocity itself $F_D \sim \nu \rho U$. While for large R_e , the laminar boundary layer becomes unstable and then turbulent. However, the whole boundary layer does not become turbulence, only some part of it. Figure 3 gives experimentally obtained graphs showing the drag coefficient as a function of the Reynolds Number $R_e = Ud/\nu$ for a cylinder with diameter *d*. For very small R_e the drag coefficient decreases according to $C_D = 24/R_e$ (Stokes formula). The decrease in C_D continues more slowly as far as $R_e \cong 5^3$, where C_D reaches a minimum, beyond which it increases somewhat. In the range of Reynolds number 2×10^4 to 2×10^5 the C_D is almost constant ([Landau and Lifshitz(2013)]).

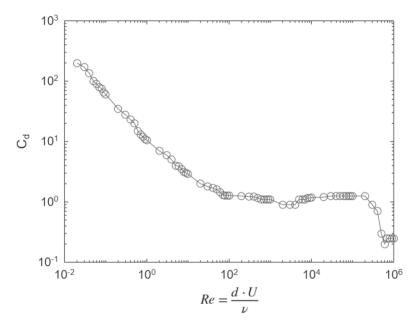


Figure 3: Experimental Plot of C_D obtained by Wieselbe ([Baracu and Boşneagu(2019)]) for varying Reynolds number

It must be borne in mind that, for the high velocities at which the drag crisis occurs, the compressibility of the fluid may begin to have a noticeable effect. The parameter which characterizes the extent of this effect is the Mach Number $M_a = U/c$, where *c* is the velocity of sound. If $M_a << 1$, the fluid may be regarded as incompressible. The experimental data indicate that the compressibility has in general a stabilizing effect on the flow in the laminar boundary layer. When M_a increases, it can be observed an increment of the critical value of R_e .