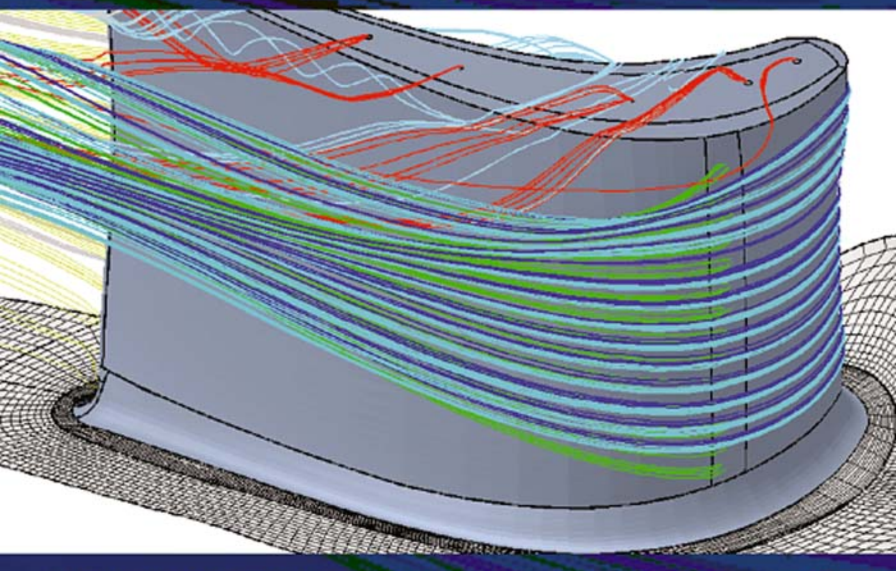
CHARLES HIRSCH

SECOND EDITION

NUMERICAL COMPUTATION OF INTERNAL & EXTERNAL FLOWS



THE FUNDAMENTALS OF COMPUTATIONAL FLUID DYNAMICS

Numerical Computation of Internal and External Flows

Volume 1

Fundamentals of Computational Fluid Dynamics

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Numerical Computation of Internal and External Flows

Volume 1
Fundamentals of Computational Fluid Dynamics

Second edition

Charles Hirsch

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To the Memory of

Leon Hirsch

and

Czypa Zugman

my parents,
struck by destiny

Contents

Preface to the second edition

This second, long (over)due, edition presents a major extension and restructuring of the initial two volumes edition, based on objective as well as subjective elements.

The first group of arguments is related to numerous requests we have received over the years after the initial publication, for enhancing the didactic structure of the two volumes in order to respond to the development of CFD courses, starting often now at an advanced undergraduate level.

We decided therefore to adapt the first volume, which was oriented at the fundamentals of numerical discretizations, toward a more self-contained and student-oriented first course material for an introduction to CFD. This has led to the following changes in this second edition:

- We have focused on a presentation of the essential components of a simulation system, at an *introductory* level to CFD, having in mind students who come in contact with the world of CFD for the first time. The objective being to make the student aware of the main steps required by setting up a numerical simulation, and the various implications as well as the variety of options available. This will cover Chapters 1–10, while Chapters 11 and 12 are dedicated to the first applications of the general methodology to inviscid simple flows in Chapter 11 and to 2D incompressible, viscous flows in Chapter 12.
- Several chapters are subdivided into two parts: an introductory level written for a first introductory course to CFD and a second, more advanced part, which is more suitable for a graduate and more advanced CFD course. We hope that by putting together the introductory presentation and the more advanced topics, the student will be stimulated by the first approach and his/her curiosity for the more advanced level, which is closer to the practical world of CFD, will be aroused. We also hope by this way to avoid frightening off the student who would be totally new to CFD, by a too 'brutal' contact with an approach that might appear as too abstract and mathematical.
- Each chapter is introduced by a section describing the 'Objectives and guidelines to this Chapter', and terminates by a section on 'Conclusions and main topics to remember', allowing the instructor or the student to establish his or her guide through the selected source material.
- The chapter on finite differences has been extended with additional considerations given to discretizations formulas on non-uniform grids.
- The chapters on finite element and finite volume methods have been merged, shifting the finite element description to the 'advanced' level, into Chapter 5 of this volume.
- A new Chapter 6 has been added devoted to an overview of various grids used in practice, including some recommendations related to grid quality.

- Chapters 7 and 8 of the first edition, devoted to the analysis of numerical schemes for consistency and stability have been merged and simplified, forming the new Chapter 7.
- Chapter 9 of the first edition has been largely reorganized, simplified and extended with new material related to general scheme properties, in particular the extremely important concept of monotonicity and the methodologies required to suppress numerical oscillations with higher order schemes, with the introduction of limiters. This is found in Chapter 8 of this volume.
- The former Chapters 10 and 11 have been merged in the new Chapter 9, devoted to the time integration schemes and to the general methodologies resulting from the combination of a selected space discretization with a separate time integration method.
- Parts of the second volume have been transferred to the first volume; in particular sections on potential flows (presented in Chapter 11) and two-dimensional viscous flows in Chapter 12. This should allow the student already to come in contact, at this introductory CFD level, with initial applications of fluid flow simulations.
- The number of problems has been increased and complete solution manuals will be made available to the instructors. Also a computer program for the numerical solutions of simple 1D convection and convection–diffusion equations, with a large variety of schemes and test cases can be made available to the instructors, for use in classes and exercises sessions. The objective of this option is to provide a tool allowing the students to develop their own 'feeling' and experience with various schemes, including assessment of the different types and level of errors generated by the combination of schemes and test cases. Many of the figures in the two volumes have been generated with these programs.

The second group of elements is connected to the considerable evolution and extension of Computational Fluid Dynamics (CFD) since the first publication of these books. CFD is now an integral part of any fluid-related research and industrial application, and is progressively reaching a mature stage. Its evolution, since the initial publication of this book, has been marked by significant advancements, which we feel have to be covered, at least partly, in order to provide the reader with a reliable and up-to-date introduction and account of modern CFD. This relates in particular to:

- Major developments of schemes and codes based on unstructured grids, which are today the 'standard', particularly with most of the commercial CFD packages, as unstructured codes take advantage of the availability of nearly automatic grid generation tools for complex geometries.
- Advances in high-resolution algorithms, which have provided a deep insight in the general properties of numerical schemes, leading to a unified and elegant approach, where concepts of accuracy, stability, monotonicity can be defined and applied to any type of equation.
- Major developments in turbulence modeling, including Direct Numerical Simulations (DNS) and Large Eddy Simulations (LES).
- Applications of full 3D Navier–Stokes simulations to an extreme variety of complex industrial, environmental, bio-medical and other disciplines, where fluids

play a role in their properties and evolution. This has led to a considerable overall experience accumulated over the last decade, on schemes and models.

- The awareness of the importance of verification and validation of CFD codes and the development of related methodologies. This has given rise to the definition and evaluation of families of test cases including the related quality assessment issues.
- The wide availability of commercial CFD codes, which are increasingly being used as teaching tools, to support the understanding of fluid mechanics and/or to generate simple flow simulations. This puts a strong emphasis on the need for educating students in the use of codes and providing them with an awareness of possible inaccuracies, sources of errors, grid and modeling effects and, more generally, with some global Best Practice Guidelines.

Many of these topics will be found in the second edition of Volume II.

I have benefited from the spontaneous input from many colleagues and students, who have been kind enough to send me notices about misprints in text and in formulas, helping hereby in improving the quality of the books and correcting errors. I am very grateful to all of them.

I also have to thank many of my students and researchers, who have contributed at various levels; in particular: Dr. Zhu Zong–Wen for the many problem solutions; Cristian Dinescu for various corrections. Benoit Tartinville and Dr. Sergey Smirnov have contributed largely to the calculations and derivations in Chapters 11 and 12.

Brussels, December 2006

Nomenclature

a	convection velocity or wave speed
A	Jacobian of flux function
c	speed of sound
c_p	specific heat at constant pressure
c_v	specific heat at constant volume
D	first derivative operator
e	internal energy per unit mass
e	vector (column matrix) of solution errors
$\vec{e}_{\mathrm{x}}, \vec{e}_{\mathrm{y}}, \vec{e}_{\mathrm{z}}$	unit vectors along the x, y, z directions
E	total energy per unit volume
E	finite difference displacement (shift) operator
f	flux function
$\vec{f}_{\mathrm{e}}$	external force vector
$\vec{\mathrm{F}}\ (f, g, h)$	flux vector with components f, g, h
g	gravity acceleration
G	amplification factor/matrix
h	enthalpy per unit mass
H	total enthalpy
I	rothalpy
J	Jacobian
k	coefficient of thermal conductivity
k	wave number
M	Mach number
n	normal distance
$\vec{n}$	normal vector
p	pressure
P	convergence or conditioning operator
Pr	Prandtl number
q	non homogeneous term
q_{H}	heat source
Q	source term; matrix of non homogeneous terms
r	gas constant per unit mass
R	residual of iterative scheme
Re	Reynolds number
s	entropy per unit mass
S	space discretization operator
$\vec{S}$	surface vector
t	time
T	temperature
u	dependent variable
U	vector (column matrix) of dependent variables

U	vector of conservative variables; velocity
$\vec{v}\ (u, v, w)$	velocity vector with components u, v, w
V	eigenvectors of space discretization matrix
$\vec{w}$	relative velocity
W	weight function
x, y, z	cartesian coordinates
z	amplification factor of time integration scheme
α	diffusivity coefficient
β	dimensionless diffusion coefficient $\beta = \alpha \Delta t / \Delta x$, also called Von Neumann number
γ	specific heat ratio
Γ	circulation; boundary of domain Ω
δ	central-difference operator
δ^+, δ^-	forward and backward difference operators
Δ	Laplace operator
Δt	time step
ΔU	variation of solution U between levels $n + 1$ and n
$\Delta x,\ \Delta y$	spatial mesh size in x and y directions
ε	error of numerical solution
ε_V	turbulence dissipation rate
ε_D	dissipation or diffusion error
ε_ϕ	dispersion error
$\vec{\zeta}$	vorticity vector
θ	parameter controlling type of difference scheme
$\vec{\kappa}$	wave-number vector; wave propagation direction
λ	eigenvalue of amplification matrix
μ	coefficient of dynamic viscosity
μ	averaging difference operator
ξ	real part of amplification matrix
η	imaginary part of amplification matrix
ρ	density; spectral radius
σ	Courant number
$\overline{\overline{\sigma}}$	shear stress tensor
$\overline{\overline{\tau}}$	stress tensor
ν	kinematic viscosity
ϕ	velocity potential; phase angle in Von Neumann analysis
Φ	phase angle of amplification factor
ω	time frequency of plane wave; overrelaxation parameters
Ω	eigenvalue of space discretization matrix; volume

Subscripts

e	external variable
i, j	mesh point locations in x, y directions
I, J	nodal point index
J	eigenvalue number

min	minimum
max	maximum
n	normal or normal component
o	stagnation values
v	viscous term
x, y, z	components in x, y, z directions; partial differentiation with respect to x, y, z
∞	freestream value

Superscripts

n	iteration level; time level

Introduction: An Initial Guide to CFD and to this Volume

Computational Fluid Dynamics, known today as ***CFD***, is defined as the set of methodologies that enable the computer to provide us with a numerical *simulation* of fluid flows.

We use the word '*simulation*' to indicate that we use the computer to solve numerically the laws that govern the movement of fluids, in or around a material system, where its geometry is also modeled on the computer. Hence, the whole system is transformed into a 'virtual' environment or *virtual product*. This can be opposed to an experimental investigation, characterized by a *material* model or prototype of the system, such as an aircraft or car model in a wind tunnel, or when measuring the flow properties in a prototype of an engine.

This terminology is also referring to the fact that we can visualize the whole system and its behavior, through computer visualization tools, with amazing levels of realism, as you certainly have experienced through the powerful computer games and/or movie animations, that provide a fascinating level of high-fidelity rendering. Hence the complete system, such as a car, an airplane, a block of buildings, etc. can be 'seen' on a computer, before any part is ever constructed.

I.1 THE POSITION OF CFD IN THE WORLD OF VIRTUAL PROTOTYPING

To situate the role and importance of CFD in our contemporary technological world, it might be of interest to take you down the road to the global world of *Computer-Assisted Engineering* or ***CAE***. CAE refers to the ensemble of simulation tools that support the work of the engineer between the initial design phase and the final definition of the manufacturing process. The industrial production process is indeed subjected to an accelerated evolution toward the *computerization of the whole production cycle*, using various software tools.

The most important of them are: Computer-Assisted Design (**CAD**), Computer-Assisted Engineering (**CAE**) and Computer-Assisted Manufacturing (**CAM**) software. The CAD/CAE/CAM software systems form the basis for the different phases of the ***virtual prototyping environment*** as shown in Figure I.1.1.

This chart presents the different components of a computer-oriented environment, as used in industry to create, or modify toward better properties, a product. This product can be a single component such as a cooling jacket in a car engine, formed by a certain number of circular curved pipes, down to a complete car. In all cases the succession of steps and the related software tools are used in very much similar ways, the difference being the degree of complexity to which these tools are applied.

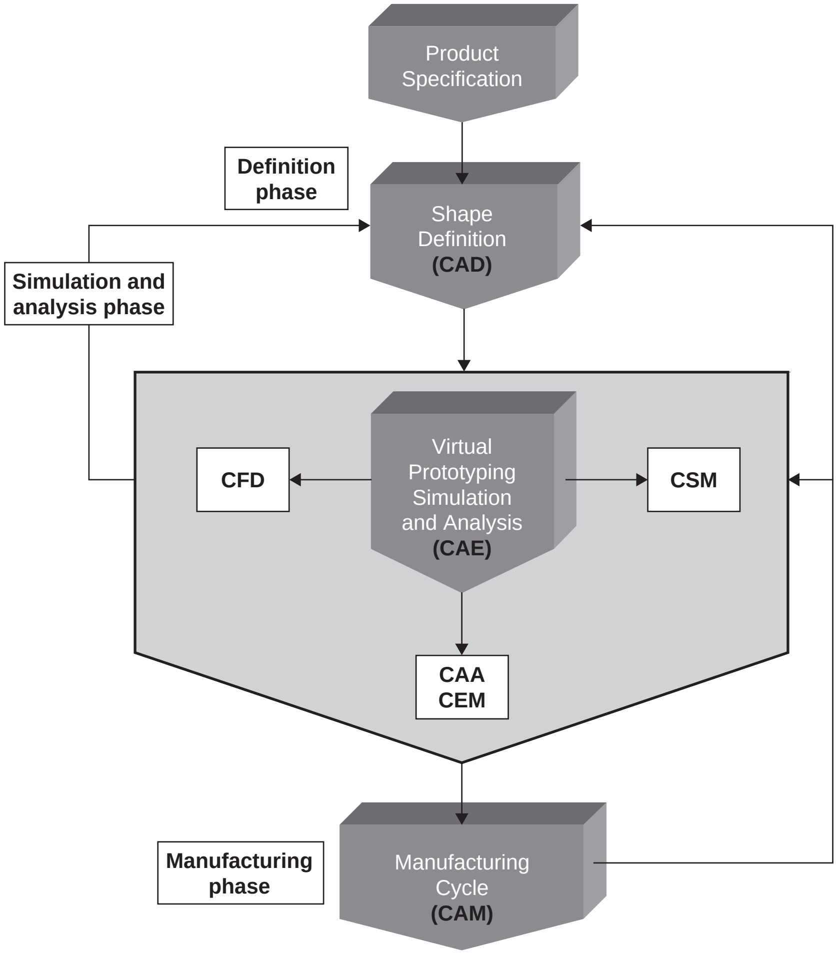


Figure I.1.1 *The structure of the virtual prototyping environment.*

I.1.1 The Definition Phase

The first step in the creation of the product is the **definition phase**, which covers the specification and geometrical definition. It is based on CAD software, which allows creating and defining the geometry of the system, in all its details. Typically, large industries can employ up to thousands of designers, working full time on CAD software. Their day-to-day task is to build the geometrical model on the computer screen, in interaction with the engineers of the simulation and analysis departments.

This CAD definition of the geometry is the required and unavoidable input to the CFD simulation task.

Figure I.1.2 shows several examples of CAD definitions of different models, for which we will see later results of CFD simulations. These examples cover a very wide range of applications, industrial, environmental and bio-medical.

Figure I.1.2a, is connected to environmental studies of wind effects around a block of buildings, with the main objective to improve the wind comfort of the people walking close to the main buildings. To analyze the problem we will have to look at the wind distribution at around 1.5 m above the ground and try to keep these wind velocities below a range of 0.5–1.0 m/s. Figure I.1.2b shows a CAD definition of an aircraft, in order to set up a CFD study of the flow around it.

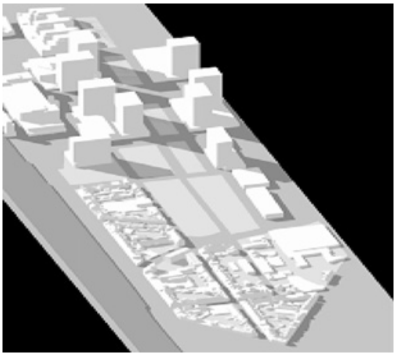
Figure I.1.2c is a multistage axial compressor, one of the components of a gas turbine engine. The objective here is to calculate the 3D flow in all the blade rows, rotors and stators of this 3.5 stage compressor, simultaneously in order to predict the performance, identify flow regions generating higher losses and subsequently modify the blading in order to reduce or minimize these loss regions.

Figure I.1.2d, from Van Ertbruggen et al. (2005), is a section of several branches of the lung and the CFD analysis has as objective to determine the airflow configuration during inspiration and to determine the path of inhaled aerosols, typical of medical sprays, in function of the size of the particles. It is of considerable importance for the medical and pharmaceutical sector to make sure that the inhaled medication will penetrate deep enough in the lungs as to provide the maximal healing effect. Finally, Figure I.1.2e and f show, respectively, the complex liquid hydrogen pump of the VULCAIN engine of the European launcher ARIANE 5 and an industrial valve system, also used on the engines of the ARIANE 5 launcher. A CFD analysis is applied in both cases to improve the operating characteristics of these components and define appropriate geometrical changes.

I.1.2 The Simulation and Analysis Phase

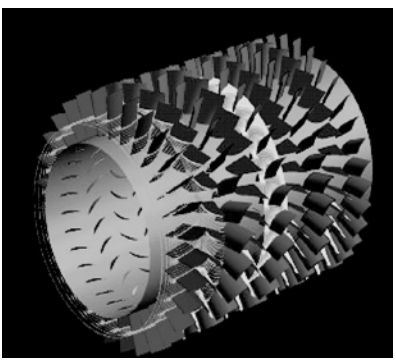
The next phase is the **simulation and analysis phase**, which applies software tools to calculate, on the computer, the physical behavior of the system. This is called *virtual prototyping*. This phase is based on CAE software (eventually supported by experimental tests at a later stage), with several sub-branches related to the different physical effects that have to be modeled and simulated during the design process. The most important of these are:

- **Computational Solid Mechanics (CSM)**: The software tools able to evaluate the mechanical stresses, deformations, vibrations of the solid parts of a system, including fatigue and eventually life estimations. Generally, CSM software will also contain modules for the thermal analysis of materials, including heat conduction, thermal stresses and thermal dilation effects. Advanced software tools also exist for simulation of complex phenomena, such as crash, largely used in the automotive sector and allowing considerable savings, when compared with the cost of real crash experiments of cars being driven into walls.
- **Computational Fluid Dynamics (CFD)**: It forms the subject of this book, and as already mentioned designates the software tools that allow the analysis of the fluid flow, including the thermal heat transfer and heat conduction effects in the fluid and through the solid boundaries of the flow domain. For instance, in the case of an aircraft engine, CFD software will be used to analyze the flow in the multistage combination of rotating and fixed blade rows of the compressor and turbine; predict their performance; analyze the combustor behavior, analyze

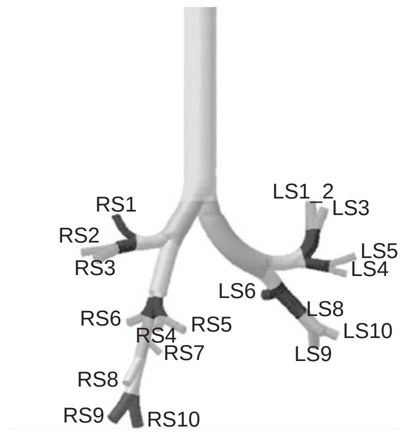


(a) Computer (CAD) model of an urban environment.

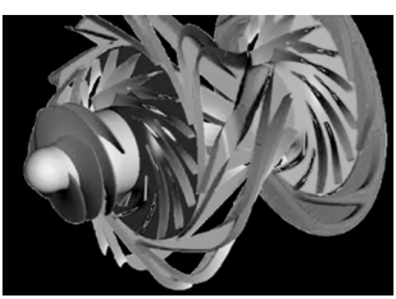
(b) Computer model (CAD) of an airplane.



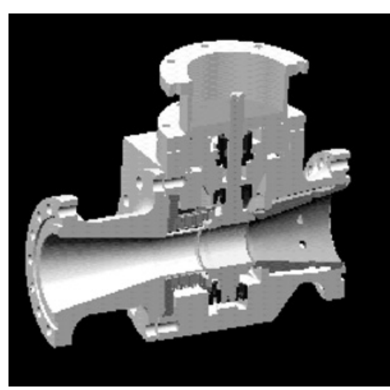
(c) Computer model of a multistage compressor.



(d) Computer model of a section of pulmonary branches in the lung. From Van Ertbruggen et al. (2005).



(e) Computer model of the liquid hydrogen pump of the VULCAIN engine of the European launcher ARIANE 5.



(f) Computer model (CAD) of an industrial valve system.

Figure I.1.2 *Examples of computer (CAD) models to initiate the steps toward a CFD simulation (for color image refer Plate I.1.2).*

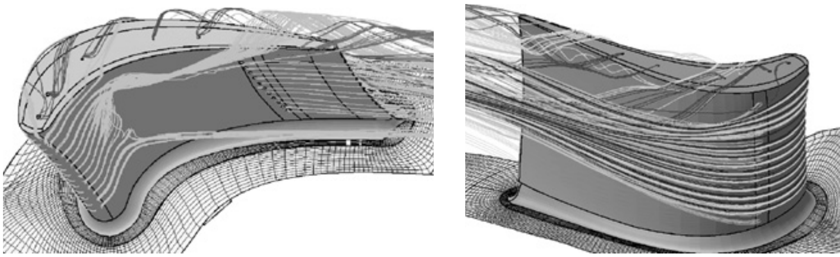


Figure I.1.3 *Simulation of the interaction between the cooling flow and the main external gas flow around a cooled turbine blade (for color image refer Plate I.1.3). Courtesy NUMECA Int. and KHI.*

the thermal parts to optimize the cooling passages, cavities, labyrinths, seals and similar sub-components. A growing number of sub-components are currently being investigated with CFD tools; while the ultimate objective is to be able to simulate the complete engine, from compressor entry to nozzle exit. An example of a complex simulation of a cooled gas turbine blade is shown in Figure I.1.3. In this simulation, the external flow around the cooled turbine interacts with the cooling flow ejected from the internal cooling passages. You can observe the very complex three-dimensional flow, which is affected by the secondary vortices, connected to the presence of the end-walls and by the tip clearance flow at the upper blade end.

- Other simulation areas related to specialized physical phenomena are also currently applied and/or in development, such as *Computational Aero-Acoustics* (CAA) and *Computational electromagnetics* (CEM). They play an important role when effects such as reduction of noise or electromagnetic interferences and signatures are important design objectives.

I.1.3 The Manufacturing Cycle Phase

In the last stage of the process, once the analysis has been considered satisfactory and the design objectives reached, **the manufacturing cycle** can start. This phase will attempt to simulate the fabrication process and verify if the shapes obtained from the previous phases can be manufactured within acceptable tolerances. This is based on the use of CAM software. This area is in strong development, as a growing number of processes are being simulated on computer, such as Forging, Stamping, Molding, Welding, for which appropriate software tools can indeed be found.

With the exploding growth of the computer hardware performance, both in terms of memory and speed, industrial manufacturers expect to simulate, in the near future, a growing number of design and fabrication processes on computer, prior to any prototype construction. This concept of *virtual product* associated to *virtual prototyping* is a major component of the technological progress, and it has already a considerable impact in all areas of industry. This impact is prone to grow further and to become a key-driving factor to all aspects of industrial analysis and design. In the automotive industry for instance, the time required for the design and production of a new car model has been reduced from 6 to 8 years in the 1970s to roughly 36 months in 2005,

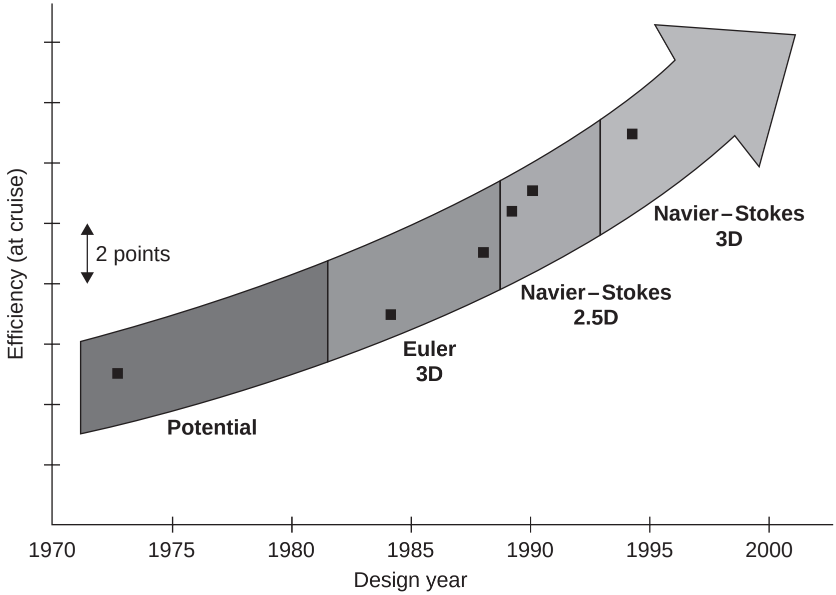


Figure I.1.4 *Impact of CFD on SNECMA fan performance, over a period of 30 years (for color image refer Plate I.1.4). From Escuret et al. (1998).*

with the announced objective of 24–18 months in the near future. A similar trend is observed in aerospace, as well as in many other highly competitive branches of industry.

It is important therefore that you realize that the major driving force behind this evolution is the wide use of computer simulations.

Coming back to the specific importance of CFD in this progress, the example of the propulsion industry is very instructive. The application of CFD has considerably improved the performance of the engines over the last 20 years, while reducing simultaneously the design cycle time. Figure I.1.4 shows the impact of the CFD tools, over a period of nearly 30 years, on the performance improvements of aircraft engines, as reported by the French engine manufacturer SNECMA. The evolution, from the initial use of simple 2D potential flow models in the early 1970s to the current applications of full 3D Navier–Stokes codes, has led to an overall gain in performance close to 10 points in efficiency. This figure also provides an interesting indication as to the period in time when the mentioned models were introduced in industry in the main design process. You will notice that 3D inviscid Euler CFD models were introduced around the mid-1980s, while the full 3D Navier–Stokes, turbulent CFD models entered the main design cycle by end of the 1990s. This evolution is due to the combination of growing computer hardware power and maturing CFD methodologies and algorithms.

A very similar impact of CFD is reported by the Boeing Company; the following statement by Boeing staff, Tinoco and Su (2004), is totally along the same line:

> *Effective use of Computational Fluid Dynamics (CFD) is a key ingredient in successful design of modern commercial aircraft. The application of CFD to*

the design of commercial transport aircraft has revolutionized the process of aerodynamic design.

Citing further from Boeing, you can find a very interesting account of 30 years of history of CFD development at this Company in Johnson et al. (2003). We highly recommend you to read this paper, as a fascinating account of how CFD evolved from an initial tool to a strategic factor in the Company's product development:

In 1973, an estimated 100 to 200 computer runs simulating flows about vehicles were made at Boeing Commercial Airplanes, Seattle. In 2002, more than 20,000 CFD cases were run to completion. Moreover, these cases involved physics and geometries of far greater complexity. Many factors were responsible for such a dramatic increase: (1) CFD is now acknowledged to provide substantial value and has created a paradigm shift in the vehicle design, analysis and support processes; … (5) computing power and affordability improved by three to four orders of magnitude …

Effective use of CFD is a key ingredient in the successful design of modern commercial aircraft. The combined pressures of market competitiveness, dedication to the highest of safety standards and desire to remain a profitable business enterprise all contribute to make intelligent, extensive and careful use of CFD a major strategy for product development at Boeing. Experience to date at Boeing Commercial Airplanes has shown that CFD has had its greatest effect in the aerodynamic design of the high-speed cruise configuration of a transport aircraft. The advances in computing technology over the years have allowed CFD methods to affect the solution of problems of greater and greater relevance to aircraft design, as illustrated in Figure 1.[1] *Use of these methods allowed a more thorough aerodynamic design earlier in the development process, permitting greater concentration on operational and safety-related features.*

The 777, being a new design, allowed designers substantial freedom to exploit the advances in CFD and aerodynamics. High-speed cruise wing design and propulsion/airframe integration consumed the bulk of the CFD applications. Many other features of the aircraft design were influenced by CFD. For example, CFD was instrumental in design of the fuselage. Once the body diameter was settled, CFD was used to design the cab. No further changes were necessary as a result of wind tunnel testing. In fact, the need for wind tunnel testing in future cab design was eliminated … As a result of the use of CFD tools, the number of wings designed and wind tunnel tested for high-speed cruise lines definition during an airplane development program has steadily decreased (Figure 3).[2]

These advances in developing and using CFD tools for commercial airplane development have saved Boeing tens of millions of dollars over the past 20 years.

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[1] See Figure I.1.5.

[2] See Figure I.1.6a. This figure shows information similar to Figure I.1.4. Figure I.1.6b shows the analogous evolution, seen from the European AIRBUS industry. We will come back to the various models mentioned in these figures in Chapter 2.

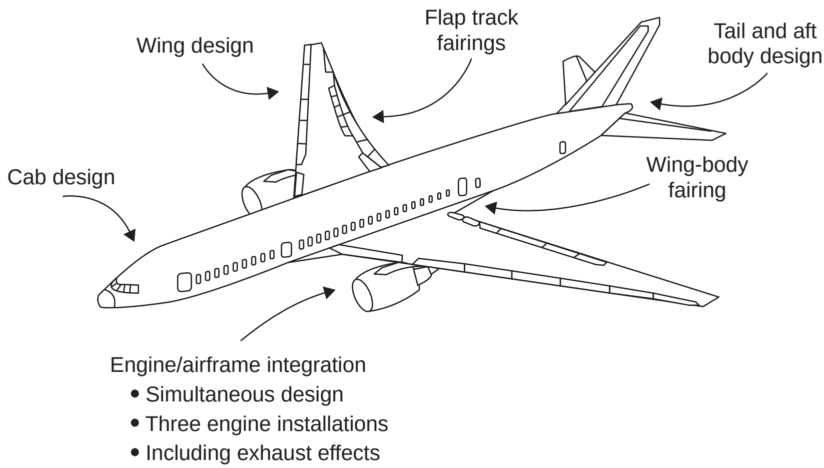


Figure I.1.5 *Role of CFD in the design of the Boeing 777. The arrows indicate the parts that were designed by CFD. From Johnson et al. (2003). Reproduced by permission of AIAA.*

> *However, significant as these savings are, they are only a small fraction of the value CFD delivered to the company.*

The following general considerations, from the same Boeing paper, confirm the strategic impact of CFD:

> *A much greater value of CFD in the commercial arena is the added value of the product (the airplane) due to the use of CFD. Value is added to the airplane product by achieving design solutions that are otherwise unreachable during the fast-paced development of a new airplane. Value is added by shortening the design development process. Time to market is critical and very important in the commercial world is getting it right the first time. No prototypes are built. From first flight to revenue service is frequently less than one year! Any deficiencies discovered during flight test must be rectified sufficiently for government certification and acceptance by the airline customer based on a schedule set years before. Any delays in meeting this schedule may result in substantial penalties and jeopardize future market success. CFD is now becoming more interdisciplinary, helping provide closer ties between aerodynamics, structures, propulsion and flight controls. This will be the key to more concurrent engineering, in which various disciplines will be able to work more in parallel rather than in the sequential manner, as is today's practice. The savings due to reduced development flow time can be enormous!*
>
> *To be able to use CFD in these multidisciplinary roles, considerable progress in algorithm and hardware technology is still necessary. Flight conditions of interest are frequently characterized by large regions of separated flows. For example, such flows are encountered on transports at low speed with deployed high-lift devices, at their structural design load conditions or when transports are subjected to in-flight upsets that expose them to speed and/or angle of attack*

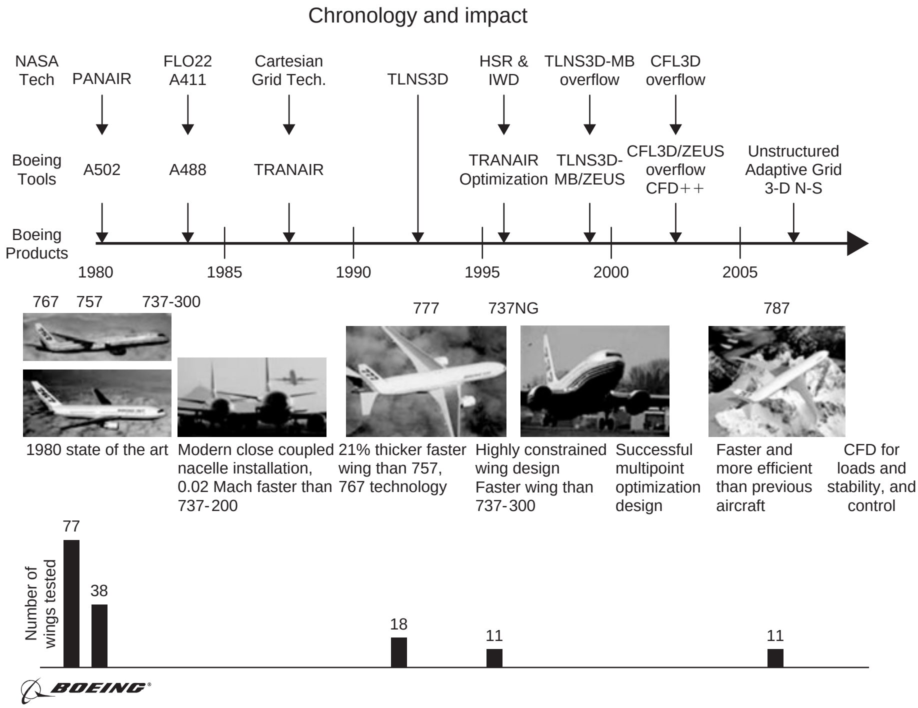


Figure I.1.6a *Evolution of the CFD tools over the last 40 years at Boeing, with an indication of the influence of CFD on the reduction of the number of wing tests (for color image refer Plate I.1.6a). Courtesy Enabling Technology and Research Organization, Boeing Commercial Airplanes.*

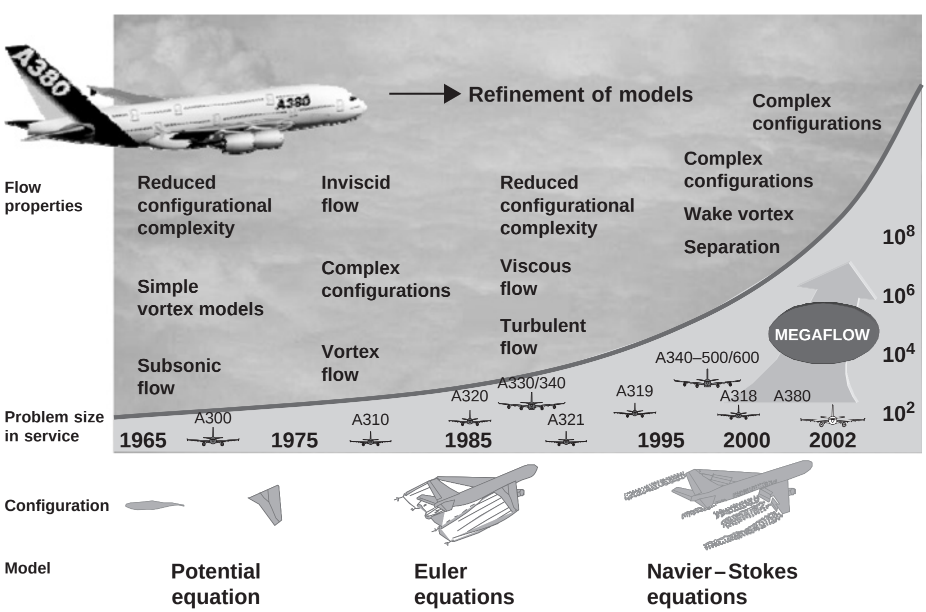


Figure I.1.6b *Evolution of the CFD tools over the last 40 years at Airbus, with an indication of the evolution of the applied models (for color image refer Plate I.1.6b). From Becker (2003).*

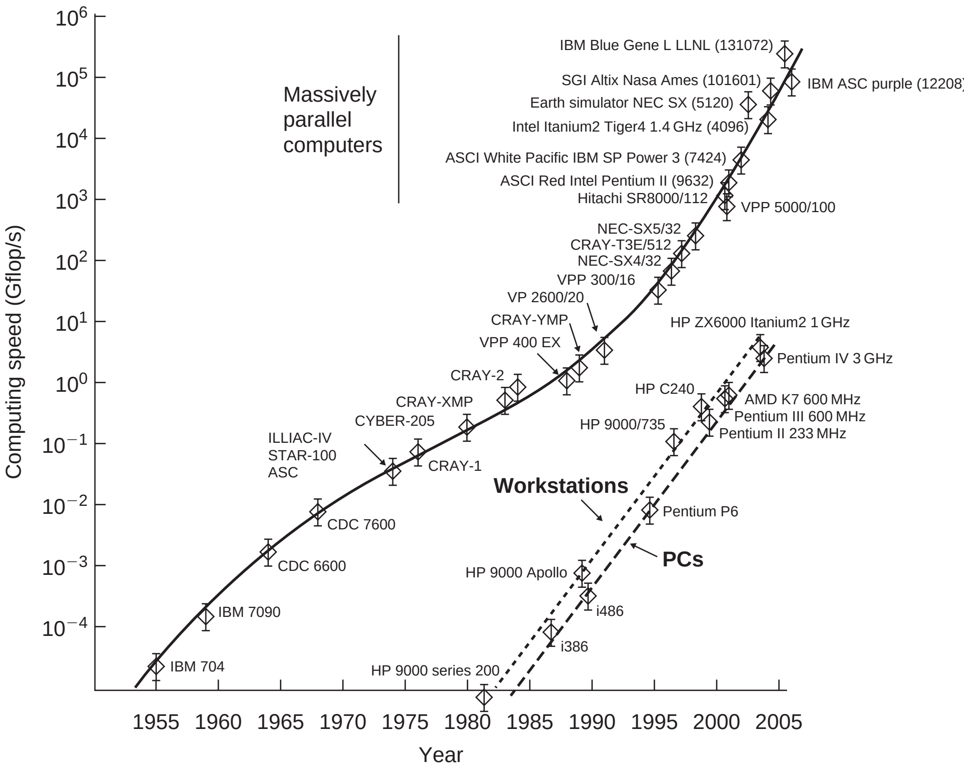


Figure I.1.7 *Evolution of Computer performance over the last 50 years, expressed in GfLOP/s, on a logarithmic scale. Courtesy Ch. Hinterberger and W. Rodi, University of Karlsruhe, Germany.*

conditions outside the envelope of normal flight conditions. Such flows can only be simulated using the Navier–Stokes equations. Routine use of CFD based on Navier–Stokes formulations will require further improvements in turbulence models, algorithm and hardware performance. Improvements in geometry and grid generation to handle complexity such as high-lift slats and flaps, deployed spoilers, deflected control surfaces and so on, will also be necessary. However, improvements in CFD alone will not be enough. The process of aircraft development, itself, will have to change to take advantage of the new CFD capabilities.

Another interesting section in this paper deals with the very important interaction between CFD and wind tunnel tests of components. We recommend you to read this section as a testimony of how CFD is contributing to raise the quality of experimental investigations.

In the previous paragraphs, we referred several times to the extraordinary growth of computing power over the last 50 years. This is summarized in Figure I.1.7, where the various computer systems are positioned by their CPU performance in function of their year of appearance. The CPU performance is measured in

GigaFlops: i.e. Billions (10^9) of floating point operations per second (Flop/s); a quite impressive number, a *Flop* being typically an addition or subtraction on the computer. The first computers in 1955 had a processor speed of 10^{-5} Gflop/s, that is of the order of 10,000 Flop/s; while the first PC with a 386 processor reached 100,000 Flop/s. Note that the level of 1000 Gflop/s, called TeraFlop/s, has been reached around the year 2000. The fastest computers shown on this figure turn around 200 TeraFlop/s, obtained through massively parallel computers over 100,000 processors. On the other hand, current high-end PCs, which are scalar computers, have a remarkable speed of the order of 5 Gflop/s.

I.2 THE COMPONENTS OF A CFD SIMULATION SYSTEM

Having positioned CFD, and its importance, in the global technological world of virtual prototyping, we should now look at the main components of a CFD system.

We wish to answer the following question: *What are the steps you have to define in order to develop, or to apply, a CFD simulation*? We make no difference at this stage between these two options, as it is similarly essential for the ‘user’ of a CFD code to understand clearly the different options available and to be able to exercise a critical judgment on all the steps involved.

Refer to Figure I.2.1 for a synthetic chart and guide to this section and the structure of this book. The CFD components are defined as follows:

- *Step 1*: It selects the mathematical model, defining the level of the approximation to reality that will be simulated (forms the content of Part I of this volume).
- *Step 2*: It covers the discretization phase, which has two main components, namely the space discretization, defined by the grid generation followed by the discretization of the equations, defining the numerical scheme (forms the content of Part II of this volume).
- *Step 3*: The numerical scheme must be analyzed and its properties of stability and accuracy have to be established (forms the content of Part III of this volume).
- *Step 4*: The solution of the numerical scheme has to be obtained, by selecting the most appropriate time integration methods, as well as the subsequent resolution method of the algebraic systems, including convergence acceleration techniques (forms the content of Part IV of this volume).
- *Step 5*: Graphic post-processing of the numerical data to understand and interpret the physical properties of the obtained simulation results. This is made possible by the existence of powerful visualization software.

Let us look at this in more details step by step.

I.2.1 Step 1: Defining the Mathematical Model

The first step in setting up a simulation is to define the physics you intend to simulate. Although we know the full equations of fluid mechanics since the second half of the 19th century, from the work of Navier and Stokes in particular, these equations are

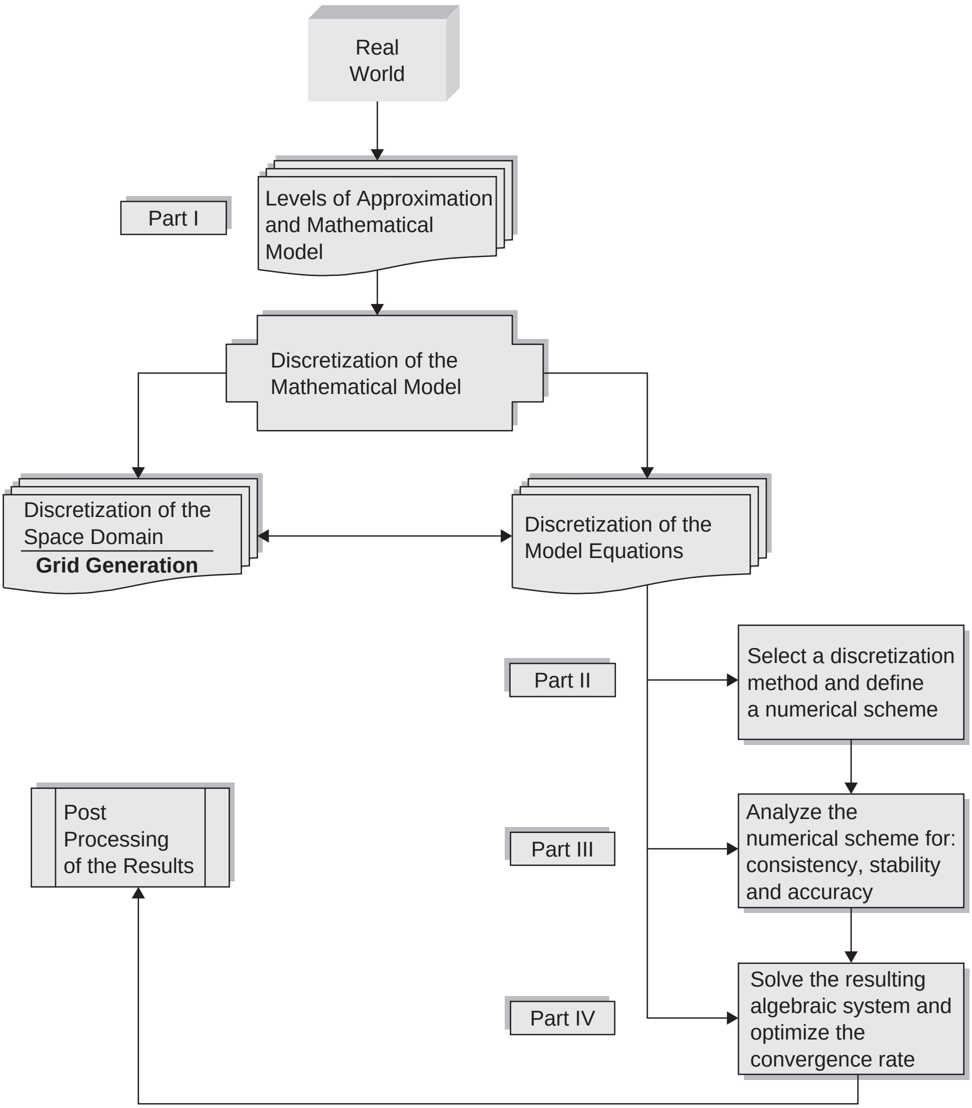


Figure I.2.1 *Structure of a CFD simulation system.*

extremely complicated. They form a system of *nonlinear* partial differential equations, with major consequences of this nonlinearity being the existence of turbulence, shock waves, spontaneous unsteadiness of flows, such as the vortex shedding behind a cylinder, possible multiple solutions and bifurcations. See Chapter 2 for some typical examples.

If we add to the basic flow more complex phenomena such as combustion, multiphase and multi-species flows with eventual effects of condensation, evaporation, bursting or agglomeration of gas bubbles or liquid drops, chemical reactions as in fire simulations, free surface flows, we need to model the physical laws describing these phenomena and provide the best possible approximations.

The essential fact to remember at this stage is that within the world of continua, as currently applied to describe the macroscopic behavior of fluids, there is ***always*** *an unavoidable level of empiricism in the models. It is therefore important that you take notice already that any modeling assumption will be associated with a generally undefined level of error when compared to the real world.*

Therefore, keep in mind that a good understanding of the physical properties and limitations of the accepted models is very important, as it is not unusual to discover that discrepancies between CFD predictions and experiments are not due to errors in experimental or numerical data, but are due to the fact that the theoretical model assumed in the computations might not be an adequate description of the real physics.

Consequently, with the exception of Direct Numerical Simulation (DNS) of the Navier–Stokes equations, we need to define appropriate modeling assumptions and simplifications. They will be translated into a mathematical model, formed generally by a set of partial differential equations and additional laws defining the type of fluid, the eventual dependence of key parameters, such as viscosity and heat conductivity in function of other flow quantities, such as temperature and pressure; as well as various quantities associated to the description of additional physics and other reactions, when present.

The establishment of adequate mathematical models for the physics to be described form the content of Part I of this volume. It is subdivided into three chapters dealing with:

- the basic flow equations (Chapter 1);
- an illustrated description of the different approximation levels that can be selected to describe a fluid flow (Chapter 2);
- the mathematical properties of the selected mathematical models (Chapter 3).

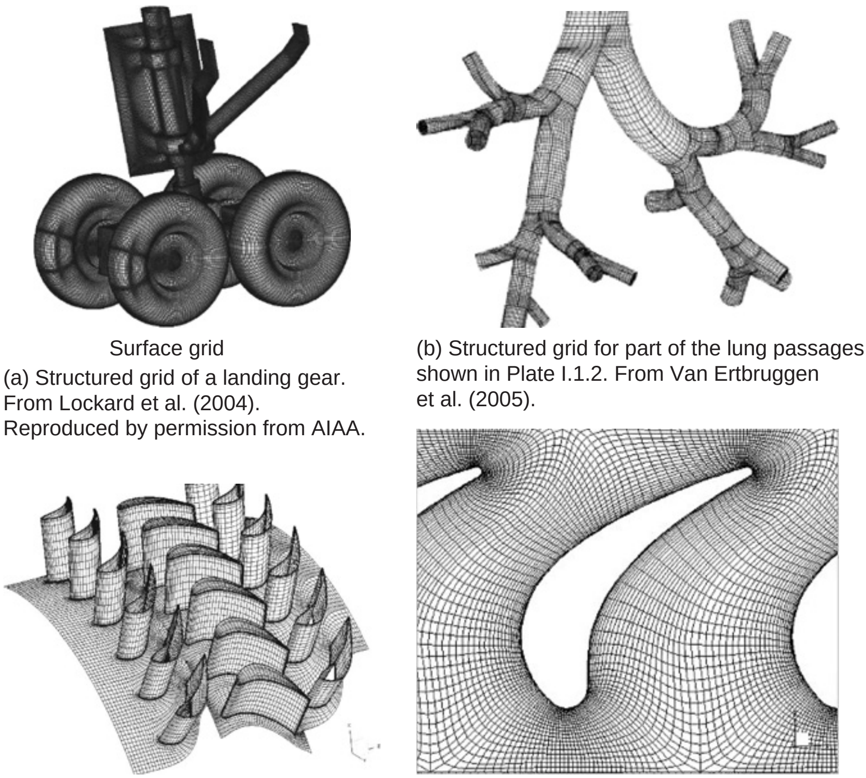
I.2.2 Step 2: Defining the Discretization Process

Once a mathematical model is selected, we can start with the major process of a simulation, namely the *discretization* process.

Since the computer recognizes only numbers, we have to translate our geometrical and mathematical models into numbers. This process is called *discretization*.

The first action is to discretize the space, including the geometries and solid bodies present in the flow field or enclosing the flow domain. The solid surfaces in the domain are supposed to be available from a CAD system in a suitable digital form, around which we can start the process of distributing points in the flow domain and on the solid surfaces. This set of points, which replaces the continuity of the real space by a finite number of isolated points in space, is called a *grid* or a *mesh*.

The process of grid generation is in general extremely complex and requires dedicated software tools to help in defining grids that follow the solid surfaces (this is called ‘body-fitted’ grids) and have a minimum level of regularity.



Surface grid
(a) Structured grid of a landing gear. From Lockard et al. (2004). Reproduced by permission from AIAA.

(b) Structured grid for part of the lung passages shown in Plate I.1.2. From Van Ertbruggen et al. (2005).

(c) Grid for a 3D turbine blade passage.

(d) Close-up view of the turbine grid.

Figure I.2.2 *Examples of structured grids.*

We will deal with the grid-related issues in Chapter 6, but we wish already here to draw your attention to the fact that, when dealing with complex geometries, the grid generation process can be very delicate and time consuming.

Grid generation is a major step in setting up a CFD analysis, since, as we will see later on, in particular in Chapters 4, 5 and 6, the outcome of a CFD simulation and its accuracy can be extremely dependent on the grid properties and quality.

Please notice here that the whole object of the simulation is for the computer to provide the numerical values of all the relevant flow variables, such as velocity, pressure, temperature, . . . , at the positions of the mesh points.

Hence, this first step of grid generation is essential and cannot be omitted. Without a grid there is no possibility to start a CFD simulation.

Figure I.2.2 shows examples of 2D and 3D *structured* grids, while Figure I.2.3 shows some examples of *unstructured* grids. These concepts will be detailed further in Chapter 6.

So, once a grid is available, we can initiate the second branch of the discretization process, namely the discretization of the mathematical model equations, as shown in the chart of Figure I.2.1.