

# An Introduction to Combustion with Applications Using Cantera

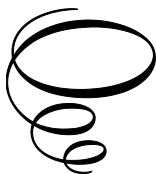


# An Introduction to Combustion with Applications Using Cantera

By

Khaled Sallam and Shubham Srivastava

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Dr. Khaled Sallam dedicates this book to his family.

Dr. Shubham Srivastava dedicates this book to his loving wife Pragya  
and his wonderful daughter Nishka.



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## PREFACE

Welcome to the fascinating world of Combustion Science. This introductory text is designed specifically with first-year graduate students and entry-level engineers in mind, particularly those tasked with performing combustion calculations as part of their professional duties. Our intention is to create a primer, a book that not only provides knowledge but also stimulates interest, instills curiosity, and fosters understanding of combustion processes and principles.

Our own journey through combustion science was enlightened by the seminal textbooks by Professors Kuo and Glassman, whose comprehensive approaches have been invaluable to the field. Their works have certainly shaped our understanding and appreciation of combustion. However, the style of this present book is markedly different. Instead of adopting a conventional textbook style, we have opted for a more interactive approach akin to lecture notes. Our purpose is to initiate a conversation about combustion. While we aim to be rigorous and thorough in our treatment of the subject, we have also strived to maintain a level of simplicity and accessibility, breaking down complex concepts into easily digestible parts.

Throughout this text, we delve into the theoretical and practical aspects of combustion, elucidating the underlying principles, mechanisms, and techniques used in combustion calculations. Each chapter is designed to not only provide essential information but also provoke thought, encouraging you to question, explore, and engage with the content in a meaningful and impactful way.

The hands-on experience in this book is based on the open-source software Cantera. A step-by-step guide to install and run Cantera is provided together with multiple examples impeded throughout the chapters. Although the experts in the field of combustion may find the information in this book elementary, they still could benefit from using the book as a Primer for the Cantera software; an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. It can be used from Python and MATLAB, or in applications written in C/C++ and Fortran 90.

Cantera is a sponsored project of NumFOCUS, a 501(c)(3) nonprofit charity in the USA. The authors of this book are not affiliated with NumFOCUS. If you find Cantera to be useful to your research or company, please consider making a donation to NumFOCUS via <https://www.cantera.org>.

As you embark on this journey, we hope that our modest contribution will serve as a useful springboard into the vast and dynamic field of combustion science. Your active participation, as you read, question, and synthesize information, will make the learning experience richer. We encourage you to embrace the stimulating challenges that lie ahead, and most importantly, enjoy the process of learning and discovery.

We wish you an enlightening and rewarding journey through the pages of this book.

*Here is a link to the repository containing files needed for a few exercises in the book –*

<https://drive.google.com/drive/folders/13GBfhTTUIWOtveYwrhZx-9t3i32P88sd?usp=sharing>

*Here are links to some video lectures on Cantera accompanying this book to enhance the learning process –*

*Introduction to Cantera*

<https://youtube.com/playlist?list=PLJjfrDRI5f4ebvIc3MZVwJHVOSh2Gg53o>

*Thermochemistry*

<https://youtube.com/playlist?list=PLJjfrDRI5f4duJB1Qd9fRVqh771g4m9mW>

*Reaction Kinetics*

<https://youtube.com/playlist?list=PLJjfrDRI5f4f45BG0a71LtEzvlOuYBXnV>

*Flames*

<https://youtube.com/playlist?list=PLJjfrDRI5f4dDhyd1v0rrnniKm0j5YB18>



# CHAPTER 1

## INTRODUCTION

### **1.1. Combustion or no combustion? That is the question!**

When you hear the word “combustion” the first thing that come to your mind may be the word “pollution”, or you may think about energy, cooking, heating, propulsion, and many other applications followed by a thought about renewable energy sources and the need to shut down all coal and gas fired power stations and to power this planet entirely using wind turbines and solar PV panels to reduce greenhouse gases and reach zero emission by 2050. Further, if you are a new engineering graduate student, you may think that you should not waste your time in graduate school on combustion courses since there will probably be no jobs in this area after you graduate. Well, nothing is further from the truth! Combustion is here to stay!

What about the combustion jobs? Combustion is currently the main technology to power our economy as shown by the 2021 U.S. energy consumption chart in Fig. 1.1. This is true now and will be true for many years to come. A quick look on the distribution of energy generation and consumption in the USA in the last 10 years would let you see how the energy sector in the USA depends on coal and natural gas and it will also make you realize that combustion will stay with us for a long time. Yes, renewable energy share is increasing every year but the change is slow to affect the position of combustion as the driver of the US economy. The sheer volume of applications involving combustion coupled with the large number of research questions that scientific community is seeking answers for, should convince you that you can find a job involving combustion after you graduate. Even with a 100% green economy, combustion will play a role in burning “green hydrogen” and fueling our hypersonic missiles and launching our rockets carrying satellites and rovers.

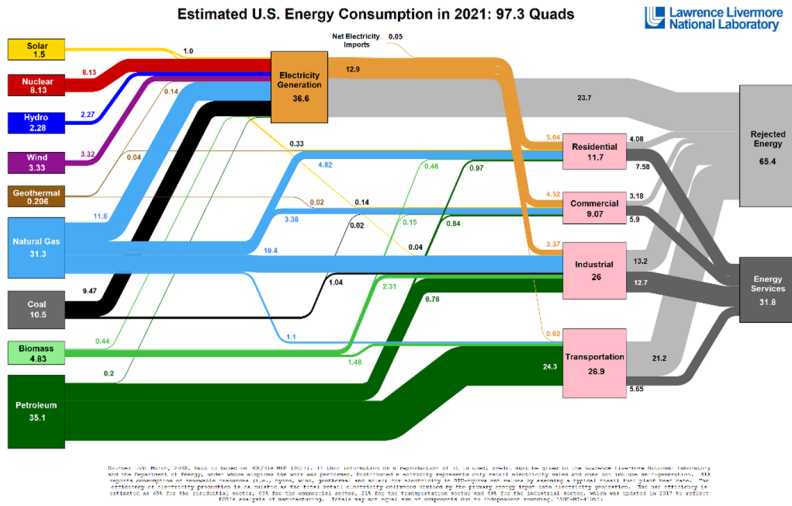


Fig. 1.1. U.S. Energy Consumption (Courtesy of Dept. of Energy).

## 1.2. Combustion Applications

Combustion started in the caves of the first humans by burning wood. It gave them heating and protected them from wild animals. It made their food more interesting. In modern days, combustion fueled the industrial revolution and gave us cars, trains, cargo ships, airplanes, and of course took us to the moon and took our rovers to Mars.

Right now, many applications could be electrified, but the affordability of natural gas in the USA makes this uneconomical in the foreseeable future, e.g. residential water and space heating in cold climates of North America. Other applications are extremely hard to electrify with our current technology e.g. *propulsion of large commercial and military planes* is among many applications that will not be electrified fully any time soon. These large cargos require powerful jet engines fueled with liquid hydrocarbon, e.g. turbo-fan engines similar to Fig. 1.2.

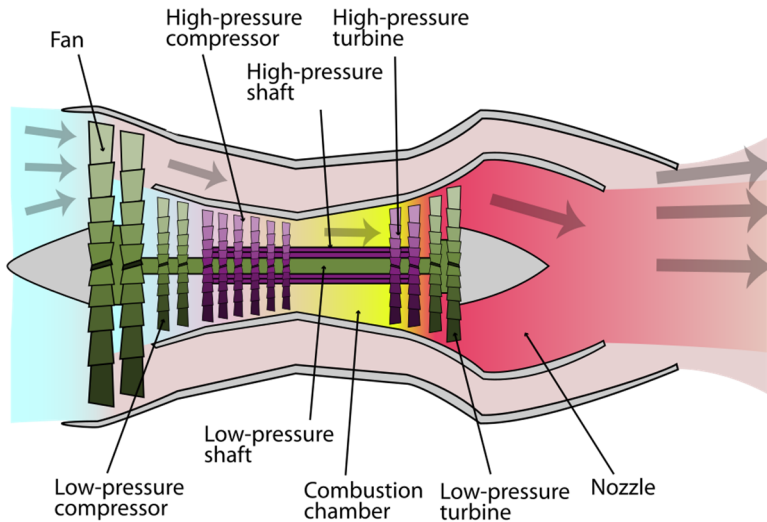


Fig. 1.2. Low Bypass Turbo Fan Jet Engine (Source [https://en.wikipedia.org/wiki/Jet\\_engine](https://en.wikipedia.org/wiki/Jet_engine)).

It is also worth noting that even with our economy fully running on renewable energy sources, there will be a need for large capacity energy storage facilities. Wind energy, currently, needs a standby guaranteed asset (e.g. natural gas fired gas turbine) to smooth the fluctuations in the energy generation profile typical of wind energy. Combustion can be used as a tool for energy storage, e.g. a future where solar energy during the summer is used to synthesis fuel (green hydrogen) for consumption during the winter is not far-fetched. At the time this book is being written, there is already a company making energy storage device that creates and consumes hydrogen fuel for residential energy applications. Sure, you can extract energy from hydrogen using fuel cells but many applications require a large amount of power that can easily be met burning hydrogen into water.

In short, combustion is here to stay. This is simply true because of propulsion and military applications that involve combustion. Think about rockets, bullets, bombs, and mines. Also, think about gas turbines, both for propulsion and power generation. It is also true because the increased energy demand we have is beyond what renewable energy industry can supply. The potential to replace batteries with green hydrogen gas turbines and using micro engine for mobile devices has motivated many researchers in the field.

### 1.3. Challenges

Indeed, combustion can cause pollution! But if you do your job correctly as an engineer the pollution would be limited and would adhere to the emission limits imposed by regulating agencies, which is getting tougher year after year locally and globally (e.g. California's rules for ultra-low NOX furnaces). You could argue back that even the cleanest combustion engine ever would still release CO<sub>2</sub> into the ambient and we should reduce green gas emission to zero. No, not entirely true, combustion engines and gas turbines burning *Hydrogen blended fuels* (e.g. syngas) could reduce CO<sub>2</sub> emission to zero if those fuels were made using carbon negative processes or using green hydrogen. Combustion can/had become a political issue. The CO<sub>2</sub> emissions are for sure increasing in the atmosphere because of industrial activities. Combustion technologies are the cause for this problem and we as engineers have to find the solution.

Improving efficiency and reducing pollution is the ultimate challenge of combustion engineers. The regulating agencies have been demanding better designs over the years, e.g. in 2022 the Biden Administration changed the 20-year-old rules for commercial water heating to eliminate non-condensing water heaters in favor of more energy-efficient condensing water heaters. Meeting new emissions targets is not always easy, e.g. lean premixed combustion reduces NO<sub>x</sub>, however, lean combustion causes thermoacoustic instabilities and new designs need to be invented to tackle both problems. The science of combustion also involves safety. This includes predicting conditions from deflagration to detonation transition.

To change current designs into more efficient and safe ones, we need robust computational simulation of combustion systems, which is very expensive computationally. The number of reactions that one needs,  $R$ , is five times the corresponding number of species involved in detailed chemistry. Accommodating realistic simulation would require a detailed prediction of turbulence-chemistry interactions as well as a complex reaction path diagram of detailed chemistry (Lu and Law, 2009). Simplified, models of the chemistry with different levels (reduced or global models) provide less accurate but more affordable simulation. A lot of efforts are devoted to the development of reduced mechanisms. Scientists evaluate those models to decide which provide reasonable solutions with affordable computational cost. The designer of a combustion system needs to be knowledgeable of combustion kinetics, thermochemistry, fluid mechanics, and heat transfer.



## 1.4. Computational Combustion

Imagine a college car racing competition where you have been entrusted with the mammoth task of designing the car that could win the race for your college and bring you laurels. You set out on this mission, making plans on how to approach the challenge. 50 years ago, your only option would be to go into a workshop, toil hard to build multiple prototypes and painstakingly test each one of them in a giant wind tunnel and eventually on a racetrack. After many such attempts you may stumble upon a good design which may not be the most optimized, but will probably get the job done. Certainly, this all sounds very cumbersome. Thankfully, computational tools come to your rescue.

Consistent developments in the discipline have ensured that there are well over 200 packages in the market claiming to be better than the rest. However, not all of them are equal. Each of them has been designed with a certain target usage. Consequently, there are specialized packages for the IC engine community, automobile aerodynamic design, combustion industry, liquids modeling and turbomachinery to name a few. They vary widely in terms of cost and capabilities. With such a wide range of choices, the decision of a software can be tough. The complexity of the challenge, the level of detail and the cost involved are few aspects that act as the guiding principles dictating the choice of the software.

All real-life problems involve analysis in the 3-dimensional space. To mimic physical processes with great accuracy a 3-dimensional treatment is preferred. However, there are many instances where achieving such a high degree of detail is rather futile and a 0 or 1 dimensional analysis may suffice. Such simulations are highly valued in the system design methodology for thermal-fluids where various components come together to forge a complete process. Here the bulk properties of the fluid, as it moves from one component to the next, are of greater importance than the thermodynamic values of the fluid at every location.

In the combustion community, Cantera and Chemkin Pro are the two most popular programs for carrying out such calculations. They specialize in performing thermodynamic calculations for laminar reacting flows which find application in simulating various flame configurations and reactor networks. Cantera is an open-source software so it can be easily accessible and modifiable but Chemkin Pro is owned by Ansys, thus restricting its distribution and access to code. In this textbook, you shall be exposed to

Cantera as a tool to conduct “numerical experiments”. A brief introduction of the package is provided in Chapter 2.

Software like Ansys Fluent, Star-CCM+ and OpenFOAM rule the roost when it comes to gaining extensive details in the 3-dimensional space with intricate physics. They provide the most comprehensive solution for the combustion community. Turbulent combustion involves complex interaction between various time and chemical scales and all this may also be accompanied with phenomena like multiphase flow, condensation, pollutant modeling and conjugate heat transfer. Handling of such broad-ranging concepts is only possible by specialized software such as these. Here again there is a distinction between the cost. Both Ansys Fluent and Star-CCM+ are commercially available software while OpenFOAM is open-source. The advantage of using an open-source software over a commercially available one is that it is freely available, modifiable and validated by various user teams around the globe. At the same time its drawbacks include lack of a support structure and a thorough knowledge of the concepts of computational methods as an absolute prerequisite. The choice is yours.

# CHAPTER 2

## COMPUTATIONAL COMBUSTION USING CANTERA

### 2.1 An introduction to Cantera

Cantera is an open-source software popular in the combustion community. The open-source movement has been of great benefit to so many of us, democratizing the knowledge and making lives easier. Cantera is the brainchild of Prof. David G. Goodwin of Caltech, a great proponent of the open-source knowledge sharing concept who made sure that the software would be available for all to use freely (Goodwin et al., 2023).

Cantera is an object-oriented software with a collection of libraries to aid solving problems in thermodynamics, transport phenomena, chemical reactions, electrochemistry, etc. The software has been written in C++ but has interfaces with C++, Python, MATLAB and Fortran along with the capability of running on multiple platforms like Windows, Mac and Linux. The development of the software began in 1998 and continues to this day where new capabilities are added with each release.

Being an open-source software, the documentation of Cantera is not at par with other commercial softwares. However, the community has done a commendable job at maintaining the software website which offers the installation package along with numerous tutorials, examples and documentation. Below are a few resources to assist a new user get started with Cantera.

Detailed documentation for Cantera is provided here:  
<https://cantera.org/>.

The Cantera website has numerous and diverse examples in Python and MATLAB along with helpful tutorials. An excellent resource for learning more about Cantera is the online forum. This is a very active community of researchers sharing ideas and resolving software-related issues faced by its members:

<https://groups.google.com/forum/embed/#!forum/cantera-users>.

## 2.2 Installing Cantera

In this section we will see detailed step by step instructions on the installation of Anaconda Python Cantera. Cantera is always undergoing development and new capabilities are continuously being added. Cantera is available for Windows, Linux and Mac and the latest version can be downloaded from the following website:

<https://cantera.org/install/index.html>.

In this book, we will focus on the Windows version with the Anaconda Python installer as it is completely open source, however, the reader can choose to use the MATLAB, Fortran, C or C++ version depending on their level of comfort with each of those platforms.

A word of caution is that this book is not intended as an instruction manual on Python language hence the expectation is that the user is proficient in the basics of Python usage.

*However, to keep matters simple very elementary level of Python has been deliberately used in this book so that readers of all Python proficiency levels can easily follow the text. Hence, the Cantera scripts in this book have been written with simplicity as the focus rather than efficiency. The reader is encouraged to explore techniques in Python to rewrite their versions of the scripts included in the text to enhance code efficiency as per their skill level.*

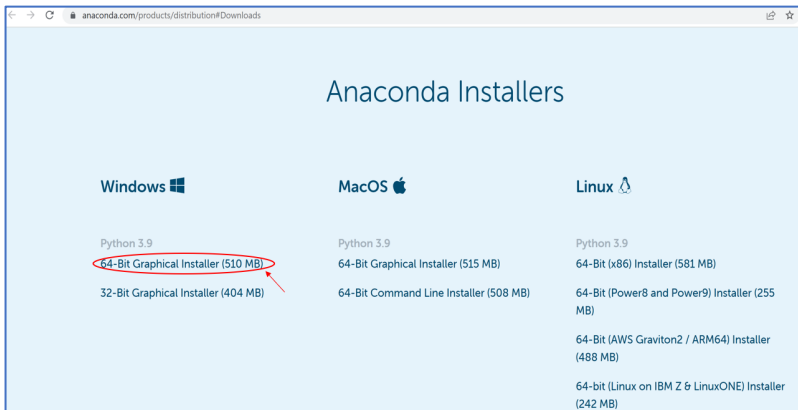
### 2.2.a Step by step instructions for Cantera installation

The instructions given in this section pertain to the installation of Cantera using the Anaconda Python distribution on the Windows platform.


Step 1 – Go to the Cantera installation website – <https://cantera.org/install/conda-install.html> – and click on the link for Anaconda Python.



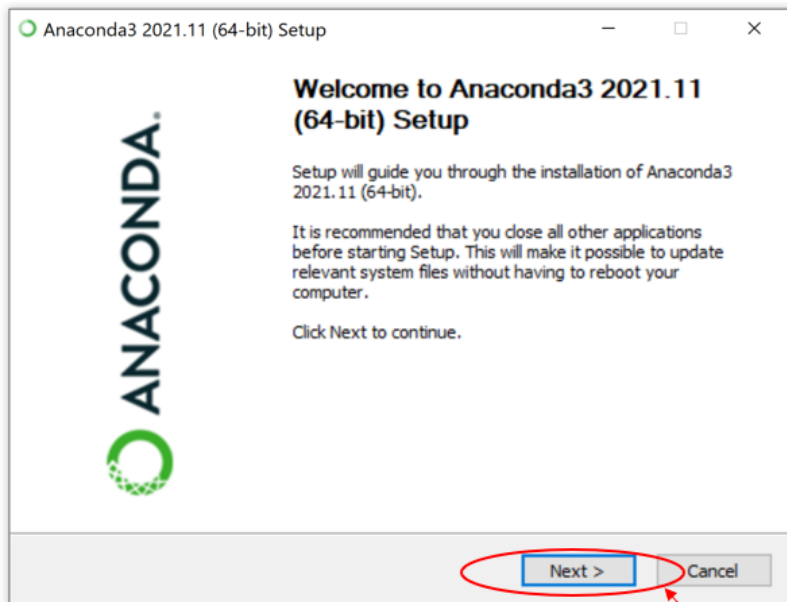
Step 2 – Download the Python installer for Windows as per your machine specifications (64 Bit or 32-Bit). Mac and Linux users can download the relevant installation files from this page also.



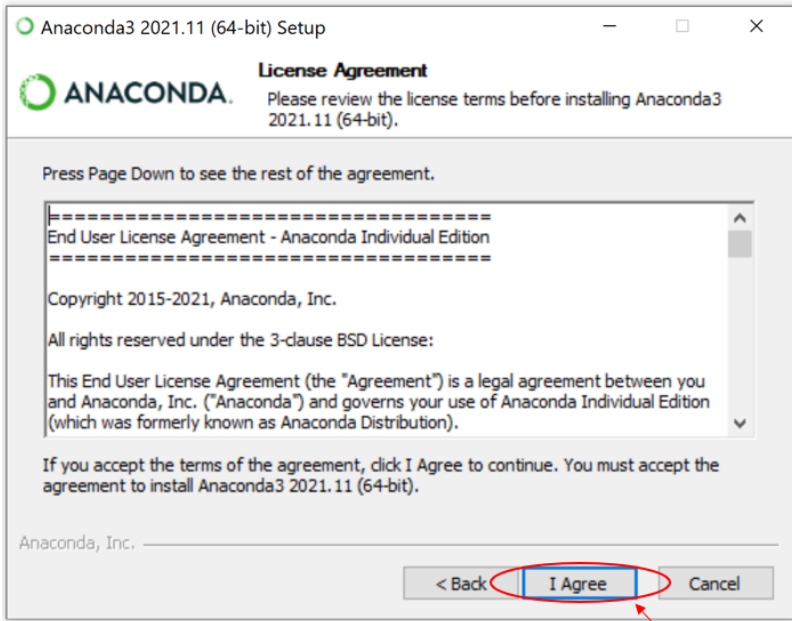
Step 3 – Run the downloaded file by clicking it.

<input type="checkbox"/> Name	Date modified	Type	Size
▼ Today (1)			
 Anaconda3-2021.11-Windows-x86_64	7/9/2022 11:30 PM	Application	522,513 KB

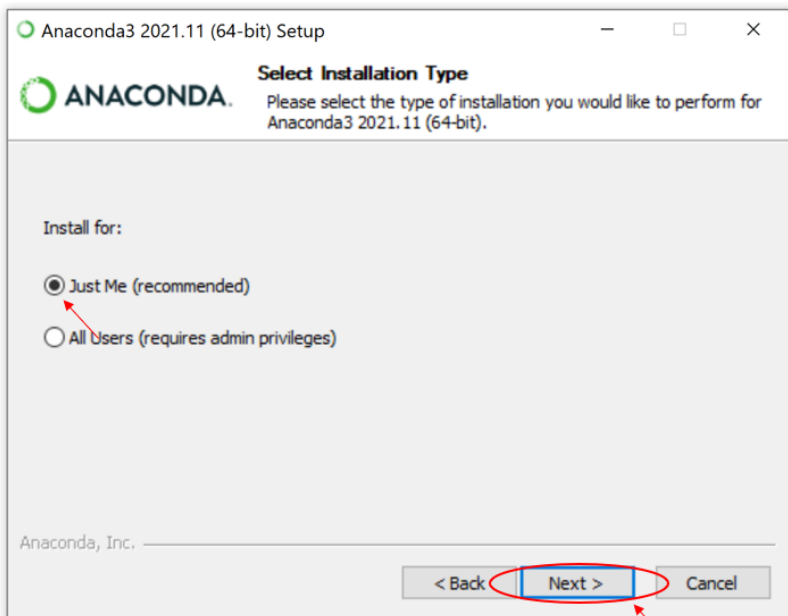
Step 4 – The set-up dialog box will appear. Click “Next” to proceed.



Step 5 – Agree to the terms of the license agreement.

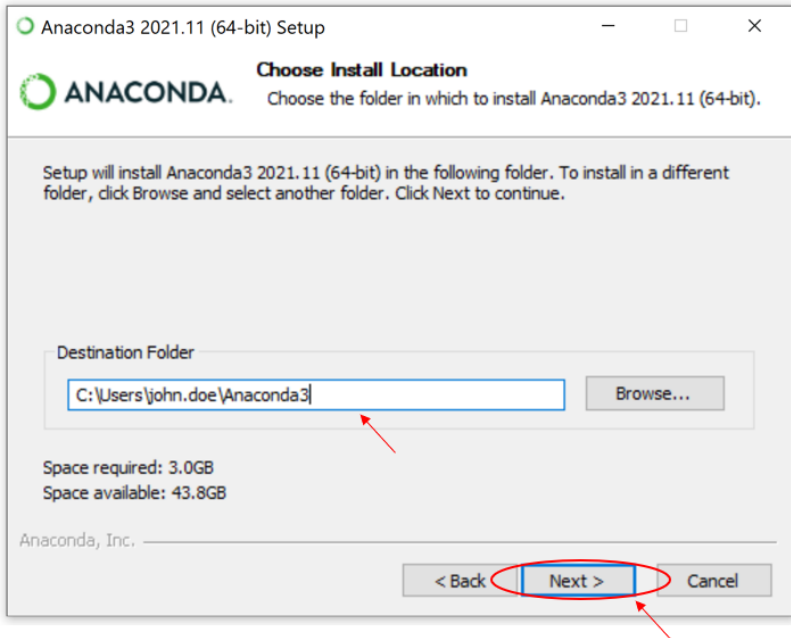


Step 6 – Select the recommended setting if setting up on a personal computer.

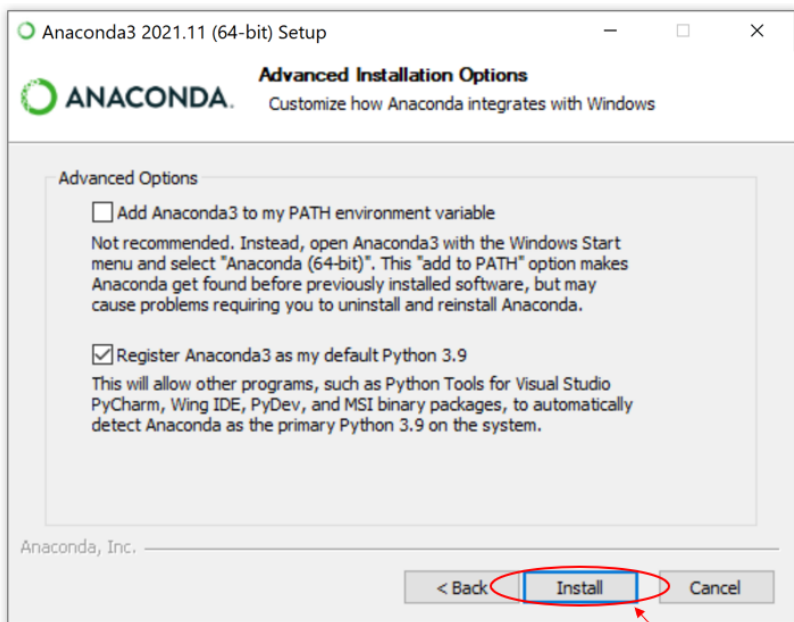




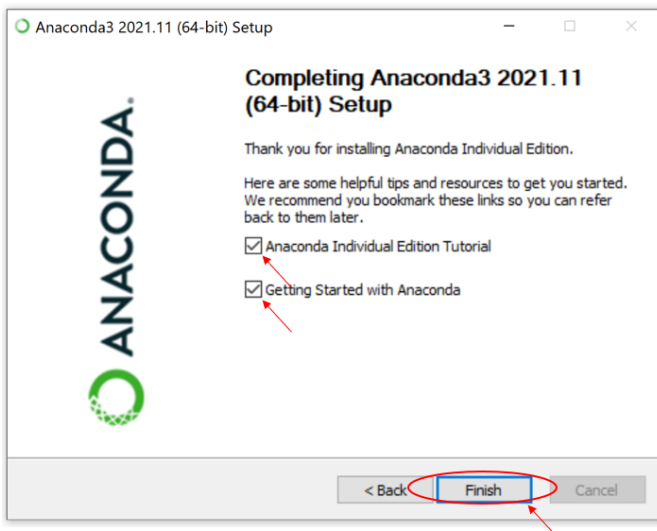
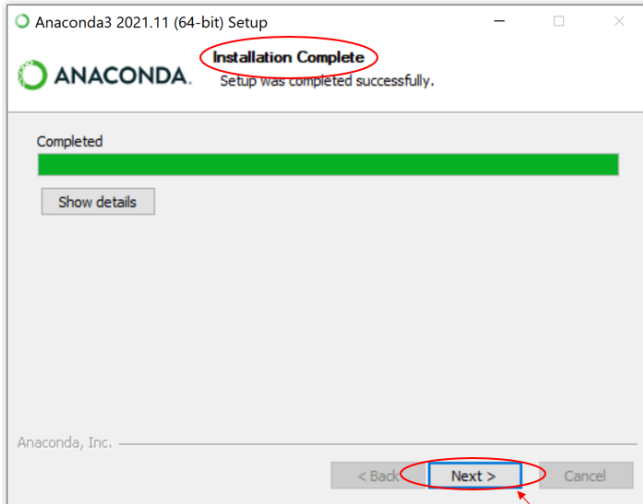
Step 7 – Enter the path of the folder where the Anaconda set up is intended.



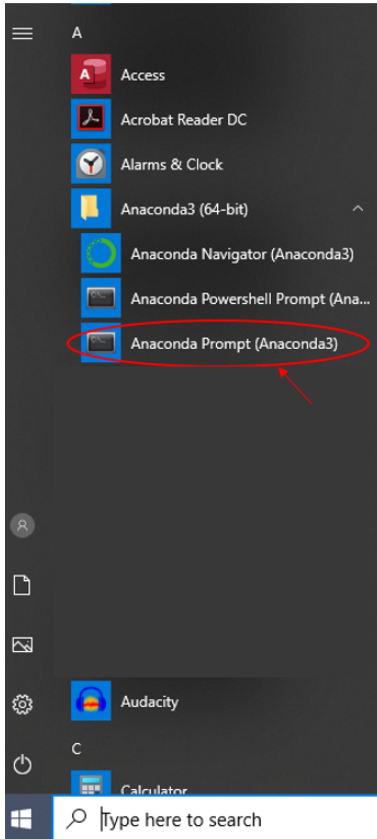
Step 8 – Accept Anaconda as the default Python.



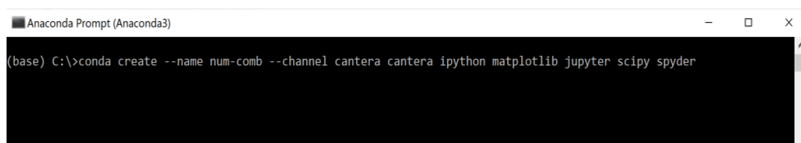
Step 9 – Wait till the installation completes. Click on the “Next” button when prompted until we arrive at the “Finish”.



Step 10 – Now that Anaconda has been successfully installed, we will install Cantera. Open the Anaconda Prompt from the Start menu.



Step 11 – At the prompt enter the command shown below. We are creating a separate environment “num-comb” in Anaconda to install Cantera and all its dependencies.



Step 12 – Press “y” when asked to proceed with the installation.

```

Anaconda Prompt (Anaconda3) - conda create --name num-comb --channel cantera cantera ipython matplotlib jupyter scipy spyder

toml          pkgs/main/noarch::toml-0.10.2-pyhd3eb1b0_0
tornado       pkgs/main/win-64::tornado-6.1-py39h2bbff1b_0
traitlets     pkgs/main/noarch::traitlets-5.1.1-pyhd3eb1b0_0
typed-ast     pkgs/main/win-64::typed-ast-1.4.3-py39h2bbff1b_1
typing_extensions pkgs/main/noarch::typing_extensions-4.1.1-hd3eb1b0_0
typing_extensions pkgs/main/noarch::typing_extensions-4.1.1-pyh06a4308_0
tzdata        pkgs/main/noarch::tzdata-2022a-hda174b7_0
ujson         pkgs/main/win-64::ujson-5.1.0-py39hd77b12b_0
unicodecode   pkgs/main/noarch::unicodecode-1.2.0-pyhd3eb1b0_0
urllib3        pkgs/main/noarch::urllib3-1.26.8-pyhd3eb1b0_0
vc            pkgs/main/win-64::vc-14.2-h21ffa51_1
vs2015_runtime pkgs/main/win-64::vs2015_runtime-14.27.29016-h5e58377_2
watchdog      pkgs/main/win-64::watchdog-2.1.6-py39haa95532_0
wcwidth       pkgs/main/noarch::wcwidth-0.2.5-pyhd3eb1b0_0
webencodings  pkgs/main/win-64::webencodings-0.5.1-py39haa95532_1
wheel         pkgs/main/noarch::wheel-0.37.1-pyhd3eb1b0_0
widgetsnbextension pkgs/main/win-64::widgetsnbextension-3.5.2-py39haa95532_0
win_inet_pton pkgs/main/win-64::win_inet_pton-1.1.0-py39haa95532_0
wincertstore  pkgs/main/win-64::wincertstore-0.2-py39haa95532_2
winpty        pkgs/main/win-64::winpty-0.4.3-4
wrapt         pkgs/main/win-64::wrapt-1.12.1-py39h196d8e1_1
xz            pkgs/main/win-64::xz-5.2.5-h62dc97_0
yaml          pkgs/main/win-64::yaml-0.2.5-hc774522_0
yapf          pkgs/main/noarch::yapf-0.31.0-pyhd3eb1b0_0
zipp          pkgs/main/noarch::zipp-3.7.0-pyhd3eb1b0_0
zlib          pkgs/main/win-64::zlib-1.2.11-hbd8134f_5
zstd          pkgs/main/win-64::zstd-1.4.9-h19a0ad4_0

Proceed ([y]/n)?

```

Step 13 – Cantera is finally installed when the following message is displayed.

```

Anaconda Prompt (Anaconda3)

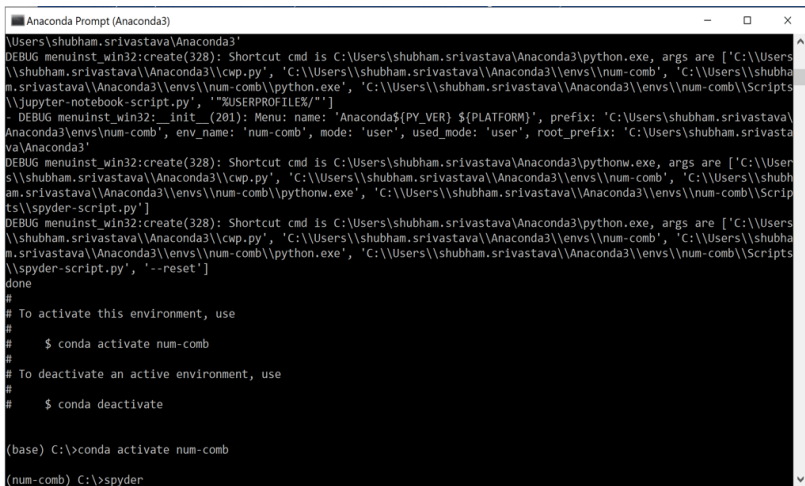
Executing transaction: / DEBUG menuinst_win32: _init_ (201): Menu: name: 'Anaconda${PY_VER} ${PLATFORM}', prefix: 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', env_name: 'num-comb', mode: 'user', used_mode: 'user', root_prefix: 'C:\Users\shubham.srivastava\Anaconda3'
DEBUG menuinst_win32:create(328): Shortcut cmd is C:\Users\shubham.srivastava\Anaconda3\python.exe, args are ['C:\Users\shubham.srivastava\Anaconda3\cwp.py', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', 'C:\Users\shubham.srivastava\Anaconda3\Scripts\python.exe', 'C:\Users\shubham.srivastava\Anaconda3\Scripts\jupyter-notebook-script.py', "%USERPROFILE%\"]
DEBUG menuinst_win32: _init_ (201): Menu: name: 'Anaconda${PY_VER} ${PLATFORM}', prefix: 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', env_name: 'num-comb', mode: 'user', used_mode: 'user', root_prefix: 'C:\Users\shubham.srivastava\Anaconda3'
DEBUG menuinst_win32:create(328): Shortcut cmd is C:\Users\shubham.srivastava\Anaconda3\python.exe, args are ['C:\Users\shubham.srivastava\Anaconda3\cwp.py', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', 'C:\Users\shubham.srivastava\Anaconda3\Scripts\python.exe', 'C:\Users\shubham.srivastava\Anaconda3\Scripts\spyder-script.py']
DEBUG menuinst_win32:create(328): Shortcut cmd is C:\Users\shubham.srivastava\Anaconda3\python.exe, args are ['C:\Users\shubham.srivastava\Anaconda3\cwp.py', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', 'C:\Users\shubham.srivastava\Anaconda3\Scripts\python.exe', 'C:\Users\shubham.srivastava\Anaconda3\Scripts\spyder-script.py', '--reset']
done

# To activate this environment, use
#
#     $ conda activate num-comb
#
# To deactivate an active environment, use
#
#     $ conda deactivate
#

(base) C:\>

```

Step 14 – Activate the newly created environment by writing command “conda activate num-comb” at the prompt as shown below. Once in the “num-comb” environment the name of the prompt will change from “base” to “num-comb”. Now start Spyder IDE by writing the command “spyder” at the “num-comb” prompt”.



```

\Users\shubham.srivastava\Anaconda3
DEBUG menuinst_win32:create(328): Shortcut cmd is C:\Users\shubham.srivastava\Anaconda3\python.exe, args are ['C:\Users\
\shubham.srivastava\Anaconda3\cwp.py', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb\python.exe', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb\Scripts
\jupyter-notebook-script.py', "%USERPROFILE%\"]
- DEBUG menuinst_win32:_init_(201): Menu: name: 'Anaconda${PY_VER} ${PLATFORM}', prefix: 'C:\Users\shubham.srivastava\
Anaconda3\envs\num-comb', env_name: 'num-comb', mode: 'user', used_mode: 'user', root_prefix: 'C:\Users\shubham.srivastava\
Anaconda3'
DEBUG menuinst_win32:create(328): Shortcut cmd is C:\Users\shubham.srivastava\Anaconda3\pythonw.exe, args are ['C:\User
s\shubham.srivastava\Anaconda3\cwp.py', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb\pythonw.exe', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb\Scripts
\spyder-script.py']
DEBUG menuinst_win32:create(328): Shortcut cmd is C:\Users\shubham.srivastava\Anaconda3\python.exe, args are ['C:\Users\
\shubham.srivastava\Anaconda3\cwp.py', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb\python.exe', 'C:\Users\shubham.srivastava\Anaconda3\envs\num-comb\Scripts
\spyder-script.py', '--reset']
done
#
# To activate this environment, use
#
#     $ conda activate num-comb
#
# To deactivate an active environment, use
#
#     $ conda deactivate
#

(base) C:\>conda activate num-comb
(num-comb) C:\>spyder

```

It will look something like this.

