# PYTHERM – INTERACTIVE COURSEWARE CONTENT FOR APPLIED THERMODYNAMICS COMPUTATIONS USING SCIENTIFIC PYTHON


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## INTRODUCTION

### 1. Why teach programming in engineering?

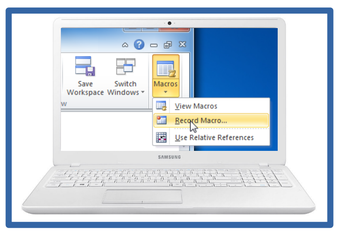



**Figure 1-a)** Task automation.


**Figure 1-b)** Improvement of calculations in parallel computing clusters.

**Figure 1-c)** Effective communication with the programming team.

**2. Context:** Many senior undergraduates and freshman graduates of the chemical engineering area show difficulty in dealing with basic assignments linked to programming.

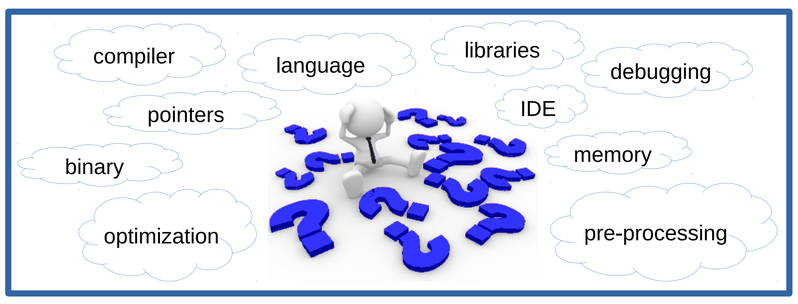



**Figure 2)** Relevant concepts.

**3. Thermodynamics:** Among the issues relevant to the formation of a professional in the field of chemical engineering, this work focuses on the area of thermodynamics, with a special focus on phase equilibrium calculations, such as petroleum, crystallization of salts, purification of biodiesel and partition of drugs between water and biological tissues[1-5].

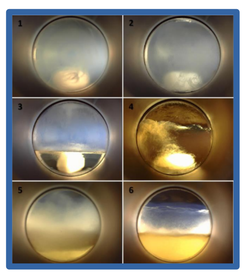


**Figure 3-a)** Phase equilibria of petroleum components.

**Figure 3-b)** Inorganic salt precipitation.


**Figure 3-c)** Phase equilibria in biodiesel production.

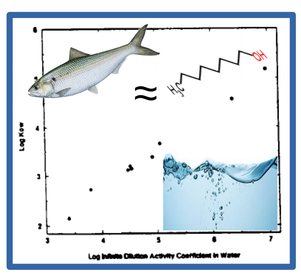



**Figure 3-d)** Partition of drugs between water in live tissues.

## OBJETIVES

**1. Interactive courseware content:** Integrating the teaching of thermodynamics to the exercise of programming, offering problems related to classes of relations and theoretical models or statistical analysis of experimental data with varying levels of programming requirement.

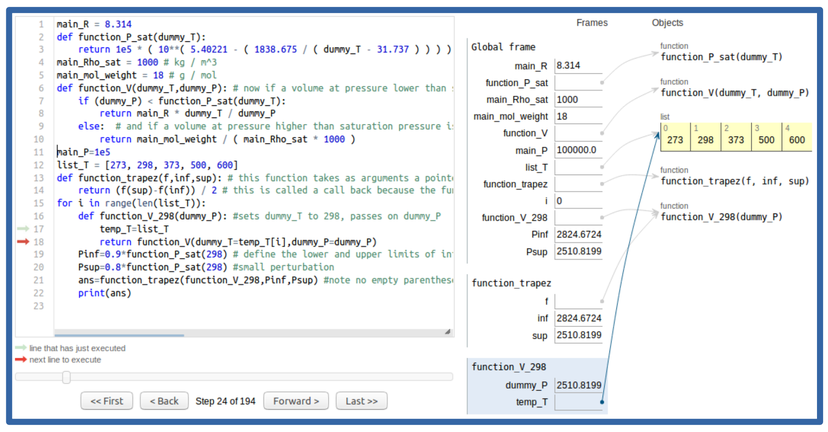
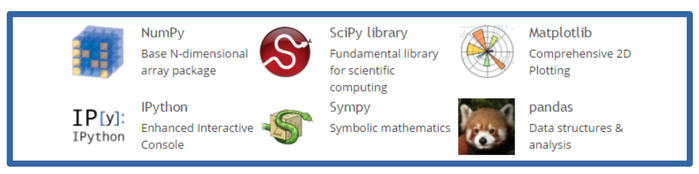



**Figure 4)** Excerpt of python 3.6 code on the Python Tutor platform exemplifying basic programming features - definition of functions and functions, scalars and lists, conditional statements and iterative loops - integrated with a motivating example of saturation pressure, volume and approximate work calculation.

## METHODOLOGY

**1. The scientific python ecosystem:** Manipulation of arrays, numerical methods, quantitative graphs, support for interactive development, symbolic calculation and statistical analysis.

**Figure 5) :** Packages in the scientific python ecosystem.




**2. Development platform:** Interactive development environment, scientific Python distribution accessible to varieties of operating system, project conversion in IPython notebook to html for static visualization in browser, web page template, remote computing server, programming logic teaching tool, hosting material and collaboration tool.

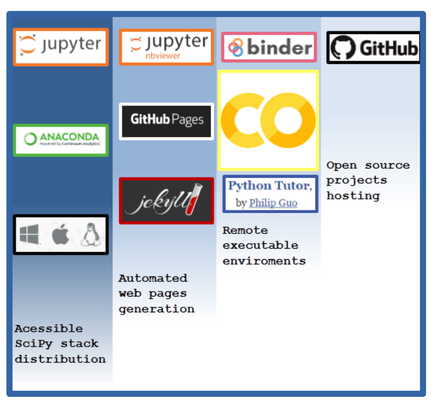



**Figure 6-a)** Tools used in the development platform.

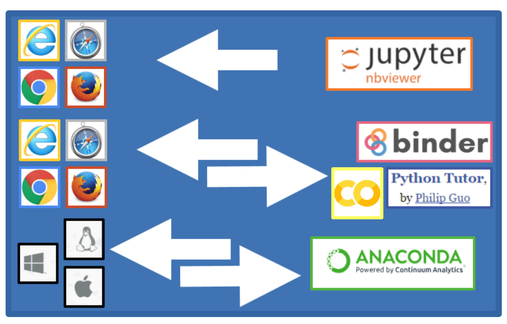



**Figure 6-b)** Tools providing acessibility in the project.

**3. Collaboration:** Open source project versioning tool, issue tracker, and collaboration.

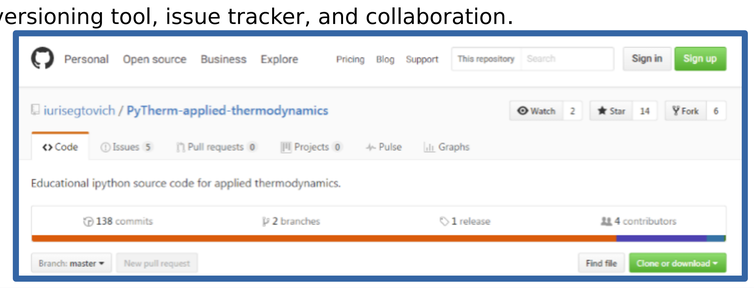
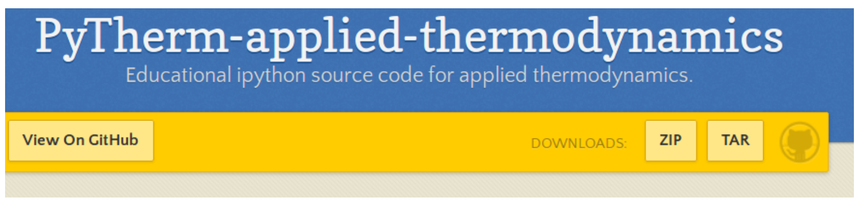



**Figure 7)** Interface of the project collaboration tool in GitHub.

## RESULTS

### 1. Webpage




**pytherm.tk**

**2. Equations of state:** Calculation of pressure as a function of volume and temperature; isopleth plots.

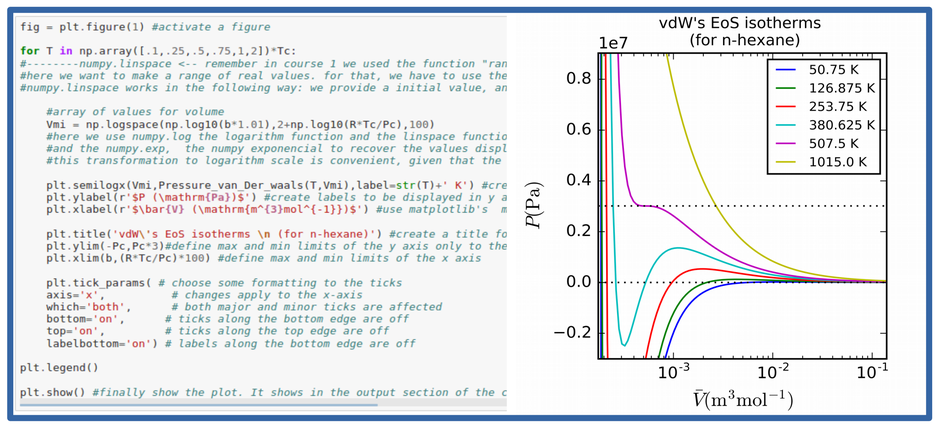



**Figure 8)** Isotherms plot of the van der Waals equation of state and excerpt of the code used.

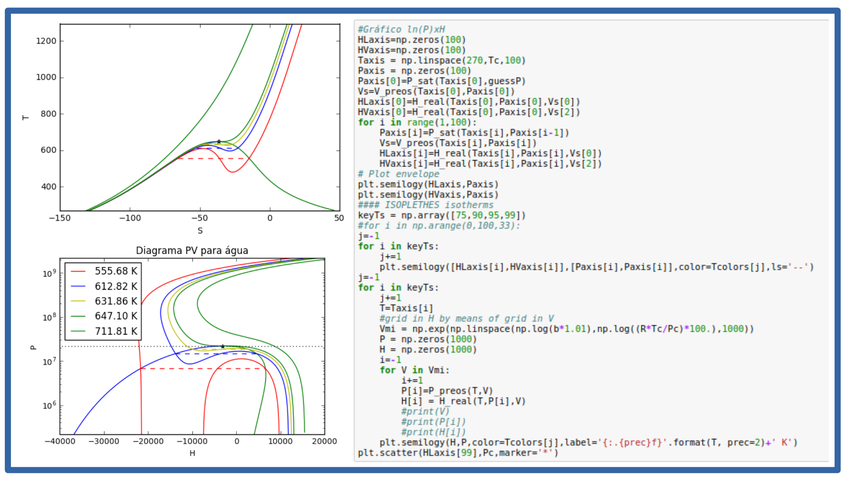



**Figure 9)** Phase envelope plots in the coordinates Pressure x Enthalpy and Temperature x Entropy for Peng-Robinson equation of state and excerpt of code used.

**3. Excess Gibbs energy models:** Calculation of excess Gibbs energy and activity coefficients as a function of temperature and composition.

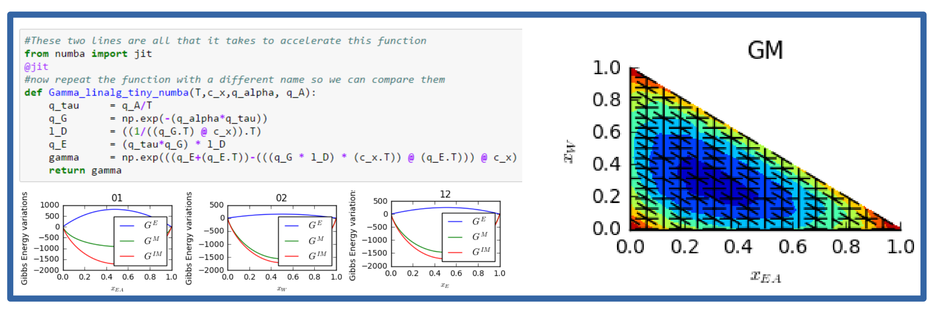
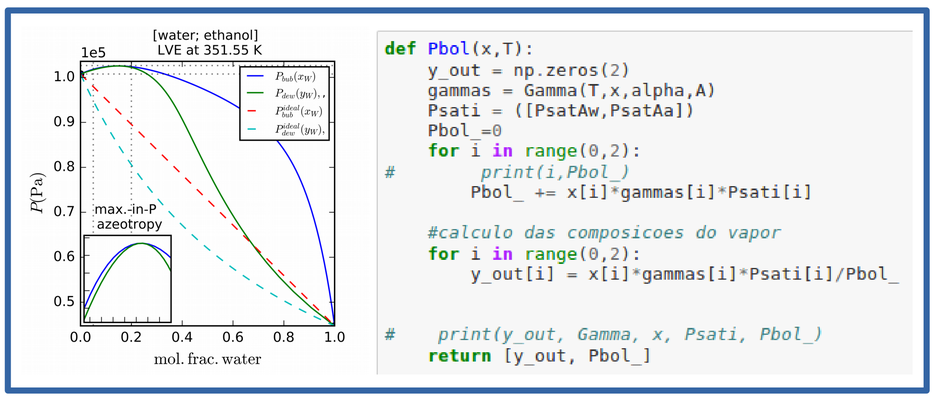



**Figure 10)** Plot of Gibbs energy of mixing from the NRTL model and excerpt from the code used.

**4. Liquid-Vapor equilibria:** Calculation of bubble and dew points in azeotropic systems.

**Figura 11)** Phase diagram of azeotropic binary system and excerpt of the code used.




**5. Liquid-Liquid equilibria:** Liquid-Liquid flash calculations.

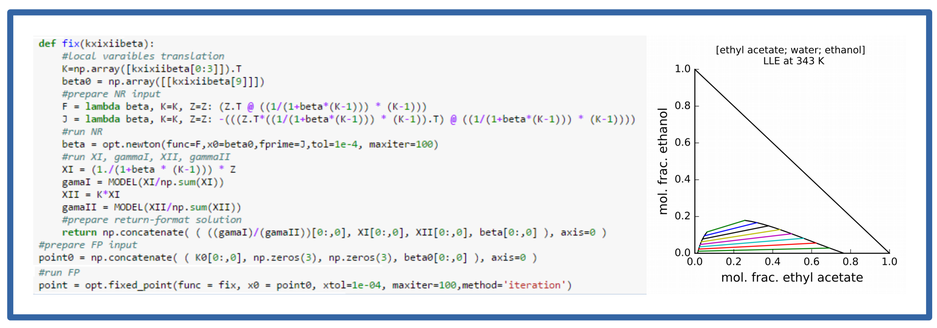



**Figura 12)** Phase diagram of ternary system and excerpt of the code used.

## CONCLUSIONS




| | Country | Sessions | % Sessions |
|---|---|---|---|
| 1. | Brazil | 159 | 49.84% |
| 2. | United States | 32 | 10.03% |
| 3. | Argentina | 15 | 4.70% |
| 4. | Czechia | 15 | 4.70% |
| 5. | Ireland | 13 | 4.08% |
| 6. | Russia | 10 | 3.13% |
| 7. | Germany | 8 | 2.51% |
| 8. | India | 7 | 2.19% |
| 9. | Italy | 7 | 2.19% |
| 10. | Australia | 5 | 1.57% |


### REFERENCES

### ACKNOWLEDGMENTS


COPPETEC, anp, PETROBRAS, CNPq, FAPERJ, CAPES

References for the figures:

- Fig 1-b) FROM <www.coppe.ufrj.br/pt-br/planeta-coppe-noticias/noticias/coppe-inaugura-o-supercomputador-lobo-carneiro> IN < http://www.coppe.ufrj.br/sites/default/files/foto_principal_400.jpg >
- Fig 1-c) FROM <www.knowledgecity.com/> IN < https://cdn0.knowledgecity.com/opencontent/courses/previews/BUS1200.jpg >
- Fig 3-a) FROM "Braga A. J. O., 2016, EQUILÍBRIO DE FASES A ALTA PRESSÃO DE SISTEMAS CONSTITUÍDOS POR CO2, FENANTRENO, TOLUENO E METANOL: ESTUDO EXPERIMENTAL, M.Sc dissertation", IN <http://tpqb.eq.ufrj.br/download/equilibrio-de-fases-a-alta-pressao-de-sistemas-constituidos-por-co2-fenantreno.pdf>
- Fig 3-b) FROM <www.acpaegypt.com/scale-inhibitors--paraffin-dispersant.html> IN <http://www.acpaegypt.com/uploads/1/0/6/7/10673668/3129251_orig.jpg>
- Fig 3-c) FROM <www.utahbiodieselsupply.com/biodieselarticles.php> IN <https://www.utahbiodieselsupply.com/images/biodieselarticles/differentstagesofbiodiesel.jpg>
- Fig 3-d) BASED ON “Sandler, 1996, INFINITE DILUTION ACTIVITY COEFFICIENTS IN CHEMICAL, ENVIRONMENTAL AND BIOCHEMICAL ENGINEERING, Fluid Phase Equilibria 116 (1996) 343-353”

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