

PyForFluids: A Python package for multicomponent fluid thermodynamic properties and phase equilibrium calculations.

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Abstract

PyForFluids (Python-Fortran-Fluids) is a Python package focused on the calculation of multicomponent fluids properties and phase equilibrium based on Equations of State (EoS). It provides a simple interface to work from a high level object oriented abstraction but also exploits the high performance Fortran code for the heavier calculations. Right now it includes the multifluid GERG-2008 EoS [1] and three cubic EoS (Peng-Robinson, Soave-Redlich-Kwong and RKPR) [2, 3, 4] are being implemented. All four equations are explicit in the Helmholtz Free Energy. PyForFluids calculates multiple thermodynamic properties like speed of sound, isobaric heat, compressibility factor, entropy, enthalpy, etc. Besides that, biphasic equilibrium calculations like flash, bubble and dew points are included, with phase envelopes tracing being in current development. To realize complex calculations, PyForFluids takes advantage of the high performance and speed of Fortran code. At the same time, it offers a user-friendly Python interface. The integration between these two programming languages is achieved thanks to numpy[5] module f2py[6]. Fortran was the chosen language due to both being faster for numerical routines and an availability of legacy projects. This package is designed with a collaborative and modular approach in mind, taking advantage of an object oriented programming approach. To both see the inner workings of it and make changes/additions proposals all the code is available on an public repository at GitHub <https://github.com/fedebenelli/pyforfluids> PyForFluids is made following programming good practices standards for continuous integration. At each code addition or modification, the package is tested with specific unit tests to assure the reliance of the computations. Also the documentation where each class and function is described is automatically generated and hosted at pyforfluids.readthedocs.io with each update, where also a simple tutorial with the basic usage of the package can be found.

Introduction

Main Objectives

1. a

Materials and Methods

Fusce magna risus, molestie ut porttitor in, consectetur sed mi. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Pellentesque consectetur blandit pellentesque. Sed odio justo, viverra nec porttitor vel, lacinia a nunc. Suspendisse pulvinar euismod arcu, sit amet accumsan enim fermentum quis. In id mauris ut dui feugiat egestas. Vestibulum ac turpis lacinia nisl commodo sagittis eget sit amet sapien.

Mathematical Section

Nulla vel nisl sed mauris auctor mollis non sed.

$$E = mc^2 \quad (1)$$

Curabitur mi sem, pulvinar quis aliquam rutrum. (1) edf (2) , $\Omega = [-1, 1]^3$, maecenas leo est, ornare at. $z = -1$ edf $z = 1$ sed interdum felis dapibus sem. x set y ytruem. Turpis j amet accumsan enim y -lacinia; ref k -viverra nec porttitor x -lacinia.

Vestibulum ac diam a odio tempus congue. Vivamus id enim nisi:

$$\begin{aligned} \cos \bar{\phi}_k Q_{j,k+1,t} + Q_{j,k+1,x} + \frac{\sin^2 \bar{\phi}_k}{T \cos \bar{\phi}_k} Q_{j,k+1} = \\ - \cos \phi_k Q_{j,k,t} + Q_{j,k,x} - \frac{\sin^2 \phi_k}{T \cos \phi_k} Q_{j,k} \end{aligned} \quad (2)$$

and

$$\begin{aligned} \cos \bar{\phi}_j Q_{j+1,k,t} + Q_{j+1,k,y} + \frac{\sin^2 \bar{\phi}_j}{T \cos \bar{\phi}_j} Q_{j+1,k} = \\ - \cos \phi_j Q_{j,k,t} + Q_{j,k,y} - \frac{\sin^2 \phi_j}{T \cos \phi_j} Q_{j,k}. \end{aligned} \quad (3)$$

Nulla sed arcu arcu. Duis et ante gravida orci venenatis tincidunt. Fusce vitae lacinia metus. Pellentesque habitant morbi. $A \underline{\xi} = \underline{\beta}$ Vim $\underline{\xi}$ enum nidi $3(P+2)^2$ lacinia. Id feugain A nun quis; magno.

Results

Donec faucibus purus at tortor egestas eu fermentum dolor facilisis. Maecenas tempor dui eu neque fringilla rutrum. Mauris *lobortis* nisl accumsan. Aenean vitae risus ante.

Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
Treatment 3	0.0009271	0.296

Table 1: Table caption

eros gravida tempor. Mauris feugiat elit et augue placerat ultrices. Morbi accumsan enim nec tortor consectetur non commodo. Pellentesque condimentum dui. Etiam sagittis purus non tellus tempor volutpat. Donec et dui non massa tristique adipiscing. Quisque vestibulum eros eu. Phasellus imperdiet, tortor vitae congue bibendum, felis enim sagittis lorem, et volutpat ante orci sagittis mi. Morbi rutrum laoreet semper. Morbi accumsan enim nec tortor consectetur non commodo nisi sollicitudin.

Phasellus imperdiet, tortor vitae congue bibendum, felis enim sagittis lorem, et volutpat ante orci sagittis mi. Morbi rutrum laoreet semper. Morbi accumsan enim nec tortor consectetur non commodo nisi sollicitudin. Proin sollicitudin. Pellentesque eget orci eros. Fusce ultricies, tellus et pellentesque fringilla, ante massa luctus libero, quis tristique purus urna nec nibh.

Nulla ut porttitor enim. Suspendisse venenatis dui eget

PLACEHOLDER
L O G O

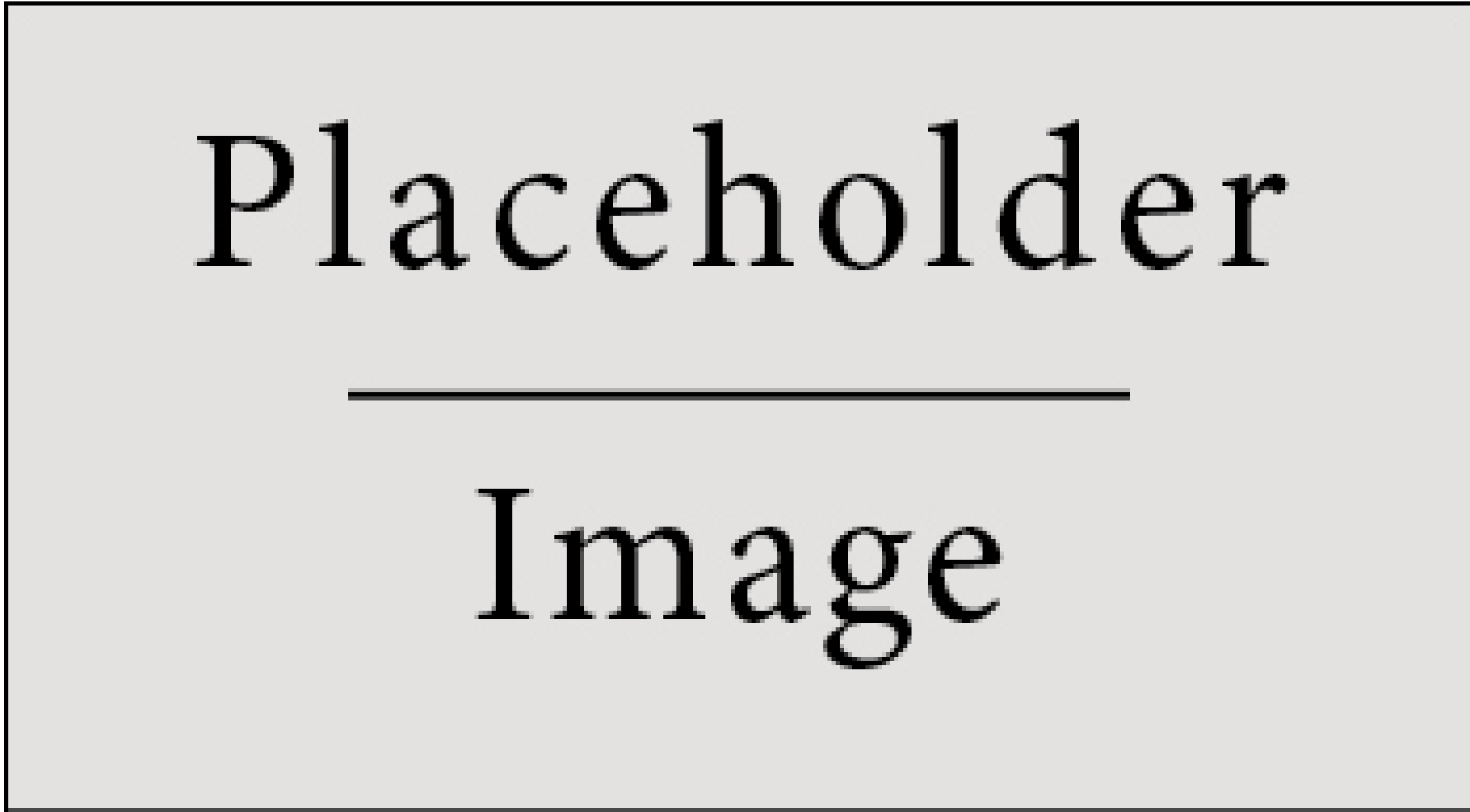


Figure 1: Figure caption

In hac habitasse platea dictumst. Etiam placerat, risus ac. Adipiscing lectus in magna blandit:

Treatments	Response 1	Response 2
Treatment 1	0.0003262	0.562
Treatment 2	0.0015681	0.910
Treatment 3	0.0009271	0.296

Table 2: Table caption

Vivamus sed nibh ac metus tristique tristique a vitae ante. Sed lobortis mi ut arcu fringilla et adipiscing ligula rutrum. Aenean turpis velit, placerat eget tincidunt nec, ornare in nisl. In placerat.

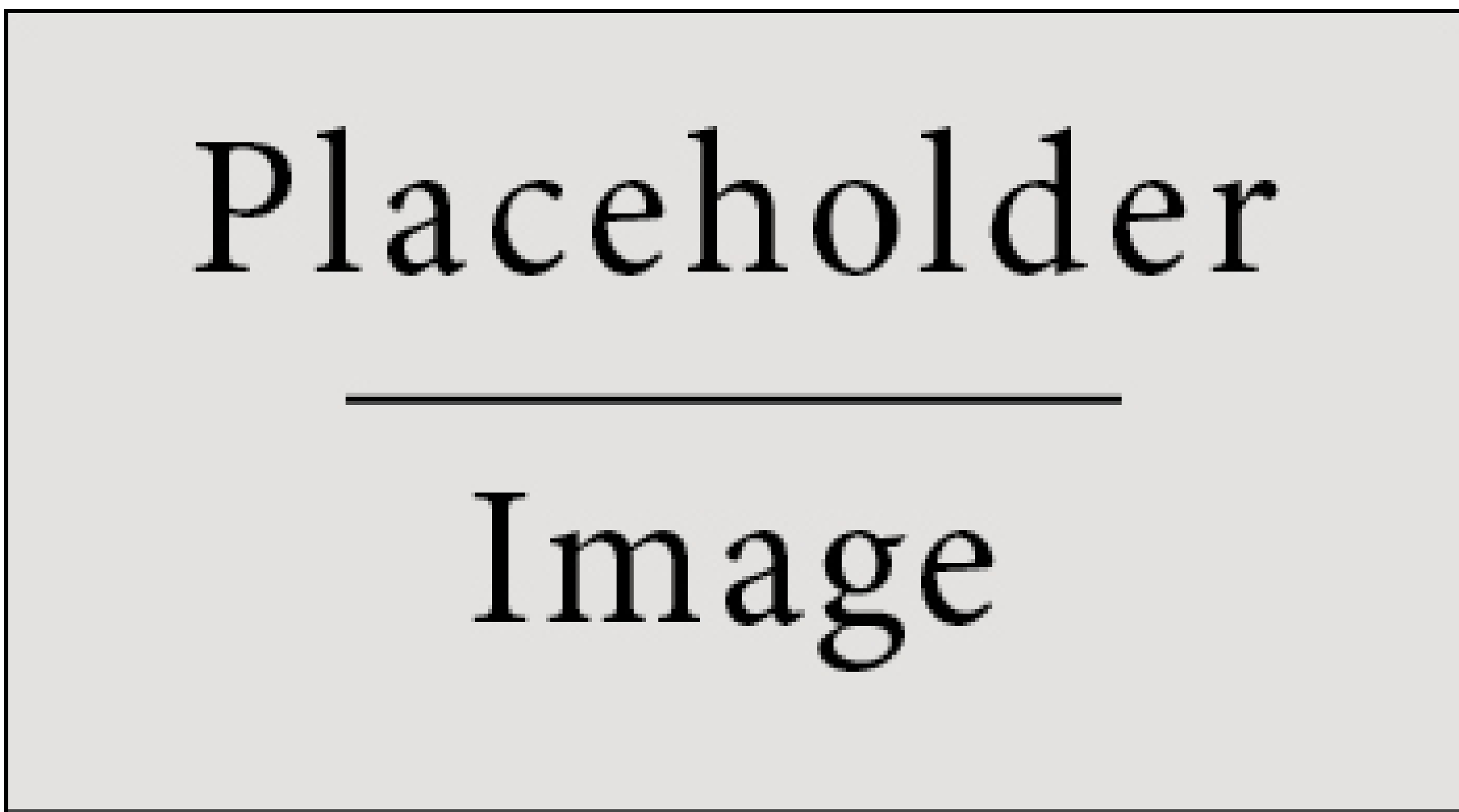


Figure 2: Figure caption

Conclusions

- Pellentesque eget orci eros. Fusce ultricies, tellus et pellentesque fringilla, ante massa luctus libero, quis tristique purus urna nec nibh. Phasellus fermentum rutrum elementum. Nam quis justo lectus.
- Vestibulum sem ante, hendrerit a gravida ac, blandit quis magna.
- Donec sem metus, facilisis at condimentum eget, vehicula ut massa. Morbi consequat, diam sed convallis tincidunt, arcu nunc.
- Nunc at convallis urna. isus ante. Pellentesque condimentum dui. Etiam sagittis purus non tellus tempor volutpat. Donec et dui non massa tristique adipiscing.

Forthcoming Research

Vivamus molestie, risus tempor vehicula mattis, libero arcu volutpat purus, sed blandit sem nibh eget turpis. Maecenas rutrum dui blandit lorem vulputate gravida. Praesent venenatis mi vel lorem tempor at varius diam sagittis. Nam eu leo id turpis interdum luctus a sed augue. Nam tellus.

References

- [1] A. B. Jones and J. M. Smith. Article Title. *Journal title*, 13(52):123–456, March 2013.
- [2] J. M. Smith and A. B. Jones. *Book Title*. Publisher, 7th edition, 2012.

Acknowledgements

Etiam fermentum, arcu ut gravida fringilla, dolor arcu laoreet justo, ut imperdiet urna arcu a arcu. Donec nec ante a dui tempus consectetur. Cras nisi turpis, dapibus sit amet mattis sed, laoreet.