modernizing PHCpack through phcpy

Jan Verschelde∗†

1 INTRODUCTION

Our mathematical problem is to solve a system of polynomial equations in several variables. The discrete part of the output data includes the number of solutions and degrees of positive dimensional solution sets. When the input is exact or if the coefficients of the polynomial can be given with any accuracy, the isolated solutions can be then approximated up to any accuracy and for each positive dimensional solution component, as many generic points as its degree can be computed.

Version 1.0 of PHCpack was archived in [Ver99]. PHCpack incorporates two external software packages: MixedVol [GLW05] and QDlib [HLB01]. Although the original focus was to approximate all isolated complex solutions, PHCpack prototyped many of the early algorithms in numerical algebraic geometry [SVW03], [SVW05]. Recent updates are listed in [Ver10].

The Python interface to PHCpack got a first start when Kathy Piret met William Stein at the software for algebraic geometry workshop at the Institute for Mathematics and its Applications in Minneapolis in the Fall of 2006. The first version of this interface is described in [Pir08]. Sage [S+13] offers the interface pcy, developed by William Stein, Marshall Hampton and Alex Jokela. Version 0.0.1 of pcy originated at lecture 40 of the author in the graduate course MCS 507 in the Fall of 2012, as an illustration of Sphinx [Bra]. Version 0.1.0 was prepared for presentation at EuroSciPy 2013 (August 2013), version 0.1.4 corresponds to the first version of this paper. The current version of pcy is 0.1.5.

We first outline in the next section the application of numerical homotopy continuation methods to compute, over the complex numbers, all isolated solutions and all positive dimensional irreducible solution sets of a polynomial system.

Then we describe how pcy relates to other interfaces to PHCpack. The functionality of pcy is then summarized briefly as the online Sphinx documentation is more extensive and still growing. The Python interface to PHCpack builds directly on the C interface to the Ada code.

Related software packages that apply homotopy continuation methods to solve polynomial systems are (in alphabetical order): Bertini [BHSW], [BHSW08], HOMPACK90 [WSM+97] (the successor of HOMPACK [WB87]), HOM4PS [GLL02], HOM4PS-2.0 [LLT08], NAG4M2 [Ley11], PHOM [GKK+04], and pss3.0.5 [Mal]. As polynomial homotopy continuation methods involve many algorithms from various fields of computing, every software has its unique strengths and the statement “no one package provides all such capabilities” quoted from [BHSW08] remains true today.

2 POLYNOMIAL HOMOTOPY CONTINUATION

Our mathematical problem is to solve a polynomial system $f(x) = 0$ in several variables $x = (x_1, x_2, \ldots, x_n)$. A homotopy connects $f(x) = 0$ to a system $g(x) = 0$ with known solutions:

$$h(x,t) = \gamma(1-t)g(x)+tf(x) = 0, \quad \gamma \in \mathbb{C}.$$ 

For almost all values for $\gamma$, the solutions of $h(x,t) = 0$ are regular for all $t \in [0,1]$. Numerical continuation methods track solution paths defined by $h(x,t) = 0$.

For systems with natural parameters $\lambda$, we solve $f(\lambda,x) = 0$ first for generic values of the parameters $\lambda = \lambda_0$ and then use

$$h(x,t) = (1-t)f(\lambda_0,x)+tf(\lambda_1,x) = 0,$$

to solve a specific instance $f(\lambda_1,x) = 0$.

The schematic in Figure 1 illustrates that singular solutions along the paths are avoided by a generic choice of the parameters $\lambda_0$ at $t = 0$.

Solving a system that has solution sets of positive dimension, e.g.: a curve or surface, means to compute its dimension and its degree. For a solution set of dimension $d$, we add to the system $d$ linear equations with random coefficients to reduce the problem to computing isolated solutions. If the dimension is not known in advance, then it can be computed in a cascade of homotopies [SV00]. Because the coefficients of the linear equation are random, the solutions of the system that satisfy the random linear equations will be isolated. If the solution set has multiplicity one, the solutions of the augmented system will be isolated points of multiplicity one. Moreover, the

Copyright © 2014 Jan Verschelde. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited. http://creativecommons.org/licenses/by/3.0/
number of isolated solutions of the augmented system that lie on the $d$-dimensional solution set of the original system will be equal to the degree of the $d$-dimensional solution set. Thus a positive dimensional solution set of dimension $d$ is represented by a set of $d$ random linear equations and as many points in the intersection of the original system with those random linear equations as the degree of the $d$-dimensional solution set. In numerical algebraic geometry, this representation is called a witness set.

For sparse polynomial systems with very few monomials appearing with nonzero coefficient (in an extreme case, we consider binomial systems that have exactly two monomials with nonzero coefficient in each equation), we can represent positive dimensional solution sets by monomial maps. For example, the two equations $x^2y - zx = 0$, $x^2z - y^2x = 0$ have as solutions three monomial maps: $(x = 0, y = \lambda_1, z = \lambda_2)$, $(x = \lambda_1, y = \lambda_2^2, z = \lambda_1^3)$, and $(x = \lambda_1, y = 0, z = 0)$, for parameters $\lambda_1$ and $\lambda_2$. These monomial maps form the leading terms of Puiseux series developments for general algebraic sets.

Surveys on homotopy continuation are [AG93], [AG97], [Li03], and [Wat02]. Book treatments are in [AG00], [Mor87], and [SW05].

3 Interfaces to PHCpack and phc

This paper is mainly concerned with software problems. There are at least three motivations to develop phcpy:

1. PHCpack is a large Ada package, its executable phc operates via menus, with input and output to files. With phcpy we provide an interpreter interface to phc.
2. The code in PHCpack lacks adequate user documentation so that many of its features are not obviously accessible to users. The Python modules of phcpy restructure the functionality of PHCpack and beautiful documentation is generated by Sphinx [Bra].
3. As many new algorithms were first implemented with PHCpack, reproducibility [SBB13] of published computational results can be automated via regression tests with Python scripts.

Because also other interfaces to PHCpack may accomplish the same goals outlined above, we first give an overview of the interfaces to PHCpack.

The first interface to PHCpack was based on the OpenXM [MNO+11] protocol for the interaction of software components. The virtue of this protocol is that only an executable version of the software is required and one does not need to compile the code.

The interfaces to PHCpack from Maple [LV04], MATLAB & Octave [GV08b], and Macaulay2 [GPV13] only require the executable phc. This type of interface works in three stages: (1) prepare an input file for phc; (2) call phc with some options, the input file, and the name of an output file; (3) parse the output file to extract the results. In principle, everything that can be done via the command-line menus of phc can thus also be performed via Maple procedures, MATLAB, Octave, or Macaulay2 scripts.

Figure 2 shows the interfaces to PHCpack.

The C interface to PHCpack, described in [LV06], offers the C programmer access to the path trackers of PHCpack. This interface was developed for use with the Message Passing Interface [SOH+98] and serves also as the basis for phcpy. In the C interface, the data structures for polynomials and solutions are not duplicated. Instead of data structure duplication, one can enter into the C interface routine a polynomial term after term. The interface then behaves like a state machine.

Why would phcpy be any better than the other interfaces? Leaving aside the growing popularity of Python for scientific computing, the replacement of files by persistent objects enabled the implementation of a generator for the path trackers. After initialization of the homotopy (with target, start system, and one start solution), the user can call a “next” function to compute the next point at the solution path that originates at the start solution given at initialization. This “next” function (available for standard double, double double, quad double precision, and arbitrary multiprecision) allows a detailed investigation of the properties of a particular solution path. In addition, it gives the user a fine control over the order
of execution. If desired, the tolerances and the step size can be adjusted as needed in an application that plots solution trajectories.

Another (future) application of phcpy is a web interface, such as at [https://kepler.math.uic.edu](https://kepler.math.uic.edu) (beta version) presented by Xiangcheng Yu at the SIAM AG 2013 conference in the first week of August 2013.

4 Using phcpy

The blackbox solver of PHCpack is its most widely used function. In phcpy, this blackbox solver is available in the function solve of the module solver. The solver takes on input a list of strings that contain valid representations of polynomials.

On return is a list of strings, which contain the solutions of the system.

```python
>>> from phcpy.solver import solve
>>> f = ['x**2*y**2 + x + y;','x*y + x + y + 1;']
>>> s = solve(f,silent=True)
```

With py2c_set_seed() we fix the seed of the random number generator for the coefficients of the start system in the homotopy, which makes for predictable runs. Otherwise, the solve() function generates different coefficients in the homotopies and the order of the solutions on return may differ. For each solution, the triplet (err,rco,res) indicates the quality of the solution:

- err: the norm of the last update made by Newton’s method (forward error),
- rco: estimate for the inverse condition number of the Jacobian matrix,
- res: norm of the evaluated solution (backward error).

With double double and quad double arithmetic we get more accurate solutions.

To predict the number of isolated solutions with the mixed volume:

```python
>>> from phcpy.solver import mixed_volume
>>> mixed_volume(f)
```

Version 0.1.5 of phcpy contains the following modules:

- solver: a blackbox solver, mixed-volume calculator, linear-product root count and start system, path trackers, deflation for isolated singular solutions.
- examples: a selection of interesting benchmark systems.
- families: some problems can be formulated for any number of variables.
- phcmaps: monomial maps as solutions of binomial systems.
- phcsols: conversion of PHCpack solution strings into Python dictionaries.
- phcsets: basic tools to manipulate positive dimensional solution sets.
- phcwulf: basic client/server setup to solve many systems.
- schubert: the Pieri homotopies solve particular polynomial systems arising in enumerative geometry.

The number of exported functions, documented by Sphinx [Bra] runs in the several hundreds. The code of version 0.1.1 of phcpy was improved with the aid of Pylint [The], yielding a global rating of 9.73/10.

5 The Design of phcpy

The design of phcpy is drawn in Figure 3. This design can be viewed as an application of a façade pattern (see Figure B.31 in [Bai08]). The façade pattern plays a strong role in converting legacy systems incrementally to more modern software and is appropriate as phcpy should be viewed as a modernization of PHCpack. The implementation of use_c2phc.adb applies the chain of responsibility pattern (see Figure B.12 in [Bai08]), calling handlers to specific packages in PHCpack. That we use the name phcpy and not PyPHC indicates that phcpy is more than just an interface.

The code for phcpy builds directly on the C interface to PHCpack. The C interface was developed to use the Message Passing Interface (MPI) [SOH+98]. In joint work with Yusong Wang [VW02], [VW04b], Yun Guan [GV08a], and Anton Leykin [LV09], [LVZ06], the main program was always a C program. The C interface described in [LV06] is centered around one gateway function use_c2phc. To the Ada programmer, this function has the specification

```ada
function use_c2phc (job : integer;
  a : C_intarrs.Pointer;
  b : C_intarrs.Pointer;
  c : C_dblarrs.Pointer )
return integer;
```
The prototype of the corresponding C function is

```c
extern int _ada_use_c2phc ( int task,
    int *a,
    int *b,
    double *c );
```

With use_c2phc we obtain one uniform streamlined design of the interface: the C programmer calls one single Ada function _ada_use_c2phc. What use_c2phc executes depends on the job number. The (a,b,c) parameters are flexible enough to pass strings and still provide some form of type checking (which would not be possible had we wiped out all types with void*).

To make _ada_use_c2phc usable, we have written a number of C wrappers, responsible for parsing the arguments of the C functions to be passed to _ada_use_c2phc. The extension module and the shared object for the implementation of phcpy is a set of wrappers defined by phcpy2c.c and documented by phcy2c.h. As a deliberate design decision of phcpy, all calls to functions in PHCpack pass through the C interface. By this design, the development of phcpy benefits the C and C++ programmers.

6 Obtaining, Installing, and Contributing

PHCpack and phcpy are distributed under the GNU GPL license (version 2 or any later version). Recently a new repository PHCpack was added on github with the source code of version 2.3.85 of PHCpack, which contains version 0.1.5 of phcpy. Executable versions for Linux, Mac, and Windows are available via the homepage of the author.

The code was developed on a Red Hat Enterprise Linux Workstation (Release 6.4) and a MacBook Pro laptop (Mac OS X 10.8.5) using the GNAT GPL 2013 compiler. Versions 2.6.6 and 2.7.3 of Python, respectively on Linux and Mac, were used to develop phcpy. Packaged binary distributions of phcpy for the platforms listed above are available via the homepage of the author.

Although the blackbox solver of PHCpack has been in use since 1996, phcpy itself is still very much in beta stage. Suggestions for improvement and contributions to phcpy will be greatly appreciated.

7 Acknowledgments

The author thanks Max Demenkov for his comments and questions at the poster session at EuroSciPy 2013. In particular the question on obtaining all solutions along a path led to the introduction of generator functions for the path trackers in version 0.1.4 of phcpy.

This material is based upon work supported by the National Science Foundation under Grant No. 1115777.

References

[AG93] E.L. Allgower and K. Georg. Continuation and path following, Acta Numerica, pages 1-64, 1993.

[AG97] E.L. Allgower and K. Georg. Numerical Path Following, in P.G. Ciarlet and J.L. Lions, editors, Techniques of Scientific Computing (Part 2), volume 5 of Handbook of Numerical Analysis, pages 3-203. North-Holland, 1997.

[AG03] E.L. Allgower and K. Georg. Introduction to Numerical Continuation Methods, volume 45 of Classics in Applied Mathematics, SIAM, 2003.

[Bai08] S.L. Bain. Emergent Design. The Evolutionary Nature of Professional Software Development, Addison-Wesley, 2008.

[BHSW] D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler. Bertini: Software for numerical algebraic geometry, available at http://www.nd.edu/~sommese/bertini.

[BHSW08] D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler. Software for numerical algebraic geometry: a paradigm and progress towards its implementation, in M.E. Stillman, N.Takayama, and J. Verschelde, editors, Software for Algebraic Geometry, volume 148 of The IMA Volumes in Mathematics and its Applications, pages 33-46, Springer-Verlag, 2008.

[Bra] G. Brandl. Sphinx: Python Documentation Generator, available at http://sphinx-doc.org.

[GLL02] T. Gao, T.Y. Li, and X. Li. HOM4PS 2.0. Proceedings of the 6th EUR. Conf. on Python in Science (EUROSCIPY 2013), volume 35 of Lecture Notes in Computer Science, pages 53-65, 2002.

[GLW05] T. Gao, T.Y. Li, and M. Wu. Algorithm 846: MixedVol: a software package for mixed-volume computation, ACM Trans. Math. Softw., 31(4):555-560, 2005.

[GKK+04] T. Gunji, S. Kim, M. Kojima, A. Takeda, K. Fujisawa, and T. Mizutani. PHoM -- a polyhedral homotopy continuation method for polynomial systems, Computing, 73(4):55-77, 2004.

[GPV13] E. Gross, S. Petrović, and J. Verschelde. PHCpack in Macaulay2, The Journal of Software for Algebra and Geometry: Macaulay2, 5:20-25, 2013.

[GV08a] Y. Guan and J. Verschelde. Parallel implementation of a subsystem-by-subsystem solver, in Proceedings of the 22th High Performance Computing Symposium, Quebec City, 9-11 June 2008, pages 117-123. IEEE Computer Society, 2008.

[GV08b] Y. Guan and J. Verschelde. PHClab: A MATLAB/Octave interface to PHCpack, in M.E. Stillman, N.Takayama, and J. Verschelde, editors, Software for Algebraic Geometry, volume 148 of The IMA Volumes in Mathematics and its Applications, pages 15-32, Springer-Verlag, 2008.

[HLB01] Y. Hida, X.S. Li, and D.H. Bailey. Algorithms for quad-double precision floating point arithmetic, in 15th IEEE Symposium on Computer Arithmetic (Arith-15 2001), 11-17 June 2001, Vail, CO, USA, pages 155-162. IEEE Computer Society, 2001. Shortened version of Technical Report LBNL-46996, software at http://crd.lbl.gov/~dhbailey/mpdist/qd-2.3.9.tar.gz.

[LLT08] T.L. Lee, T.Y. Li, and C.H. Tsai. HOM4PS-2.0: a software package for solving polynomial systems by the polyhedral homotopy continuation method, Computing, 83(2-3):109-133, 2008.

[Ley11] A. Leykin. Numerical algebraic geometry, The Journal of Software for Algebra and Geometry: Macaulay2, 3:5-10, 2011.

[LV04] A. Leykin and J. Verschelde. PHCMaple: A Maple interface to the numerical homotopy algorithms in PHCpack, in Proceedings of the Tenth International Conference on Applications of Computer Algebra (ACA’2004), pages 139-147, 2004.

[LV05] A. Leykin and J. Verschelde. Factoring solution sets of polynomial systems in parallel, in T. Skeie and C.-S. Yang, editors, Proceedings of the 2005 International Conference on Parallel Processing Workshops. 14-17 June 2005. Oslo, Norway. High Performance Scientific and Engineering Computing, pages 173-180, IEEE Computer Society, 2005.

[LV06] A. Leykin and J. Verschelde. Interfacing with the numerical homotopy algorithms in PHCpack, in N. Takayama and A. Iglezias, editors, Proceedings of ICMCS 2006, volume 4151 of Lecture Notes in Computer Science, pages 354-360, Springer-Verlag, 2006.

[LV09] A. Leykin and J. Verschelde. Decomposing solution sets of polynomial systems: a new parallel monodromy breakup algorithm, The International Journal of Computational Science and Engineering, 4(2):94-101, 2009.

[LV206] A. Leykin, J. Verschelde, and Y. Zhuang. Parallel homotopy algorithms to solve polynomial systems, in N. Takayama and A. Iglezias, editors, Proceedings of ICMCS 2006, volume 4151 of Lecture Notes in Computer Science, pages 225-234, Springer-Verlag, 2006.

[Li03] T.Y. Li. Numerical solution of polynomial systems by homotopy continuation methods, in F. Cucker, editor, Handbook of Numerical Analysis. Volume X. Special Volume: Foundations of Computational Mathematics, pages 209-304. North-Holland, 2003.

[Mal] G. Malajovich. pss3.0.5: Polynomial system solver, version 3.0.5, available at http://www.labma.ufrj.br/~gregorio/software.php.
MODERNIZING PHCPACK THROUGH PHCPY

[MNO+11] M. Maekawa, M. Noro, K. Ohara, N. Okutani, Y. Takayama, and Y. Tamura. OpenXM -- an open system to integrate mathematical softwares, 2011, available at http://www.OpenXM.org.

[Mor87] A. Morgan. Solving polynomial systems using continuation for engineering and scientific problems, Prentice-Hall, 1987. Volume 57 of Classics in Applied Mathematics Series, SIAM 2009.

[Pic08] K. Piret. Computing Critical Points of Polynomial Systems using PHCpack and Python, PhD thesis, University of Illinois at Chicago, 2008.

[SOH+98] M. Snir, S. Otto, S. Huss-Lederman, D. Walker, and J. Dongarra. MPI - The Complete Reference Volume I, The MPI Core, Massachusetts Institute of Technology, second edition, 1998.

[S+13] W.A. Stein et al. Sage Mathematics Software (Version 5.12), The Sage Development Team, 2013. http://www.sagemath.org.

[SV00] A.J. Sommese and J. Verschelde. Numerical homotopies to compute generic points on positive dimensional algebraic sets. J. of Complexity, 16(3):572-602, 2000.

[SVW03] A.J. Sommese, J. Verschelde, and C.W. Wampler. Numerical irreducible decomposition using PHCpack, in M. Joswig and N. Takayama, editors, Algebra, Geometry, and Software Systems, pages 109-130. Springer-Verlag, 2003.

[SVW05] A.J. Sommese, J. Verschelde, and C.W. Wampler. Introduction to numerical algebraic geometry, in A. Dickenstein and I.Z. Emiris, editors, Solving Polynomial Equations, Foundations, Algorithms and Applications, volume 14 of Algorithms and Computation in Mathematics, pages 301-337. Springer-Verlag, 2005.

[SW05] A.J. Sommese and C.W. Wampler. The Numerical solution of systems of polynomials arising in engineering and science, World Scientific Press, Singapore, 2005.

[SVW02] J. Verschelde and Y. Wang. Numerical homotopy algorithms for satellite trajectory control by pole placement, Proceedings of MTNS 2002, Mathematical Theory of Networks and Systems (CDROM), Notre Dame, August 12-16, 2002.

[VW04a] J. Verschelde and Y. Wang. Computing feedback laws, IEEE Transactions on Automatic Control, 49(8):1393-1397, 2004.

[VW04b] J. Verschelde and Y. Wang. Computing feedback laws for linear systems with a parallel Pieri homotopy, In Y. Yang, editor, Proceedings of the 2004 International Conference on Parallel Processing Workshops, 15-18 August 2004, Montreal, Quebec, Canada. High Performance Scientific and Engineering Computing, pages 222-229, IEEE Computer Society, 2004.

[VZ06] J. Verschelde and Y. Zhuang. Parallel implementation of the polyhedral homotopy method, In T.M. Pinkston and F. Ozguner, editors, Proceedings of the 2006 International Conference on Parallel Processing Workshops, 14-18 Augustus 2006, Columbus, Ohio, High Performance Scientific and Engineering Computing, pages 481-488, IEEE Computer Society, 2006.

[Wat86] L.T. Watson. Numerical linear algebra aspects of globally convergent homotopy methods, SIAM Rev., 28(4):529-545, 1986.

[Wat89] L.T. Watson. Globally convergent homotopy methods: a tutorial, Appl. Math. Comput., 31(Spec. Issue):369-396, 1989.

[Wat02] L.T. Watson. Probability-one homotopies in computational science, J. Comput. Appl. Math., 140(1&2):785-807, 2002.

[WBM87] L.T. Watson, S.C. Billups, and A.P. Morgan. Algorithm 652: HOMPACK: a suite of codes for globally convergent homotopy algorithms, ACM Trans. Math. Softw., 13(3):281-310, 1987.

[WSM+97] L.T. Watson, M. Sosonkina, R.C. Melville, A.P. Morgan, and H.F. Walker. Algorithm 777: HOMPACK90: A suite of Fortran 90 codes for globally convergent homotopy algorithms, ACM Trans. Math. Softw., 23(4):514-549, 1997.
