An Introduction to Asymptotic Approximants

Nate Barlow
School of Mathematical Sciences, RIT

All work done with co-conspirator of the method:
Steve Weinstein
Chemical Engineering, RIT

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Overview

In this talk, the method of *asymptotic approximants* will be applied to obtain analytic solutions for:

- an elliptic **integral** important to light bending.
- nonlinear **differential equations** of fluid dynamics.
- the analytic continuation of certain **truncated expansions** of thermodynamics and astrophysics

History of Asymptotic approximants

- 1961: Baker & Gammel's Padé Approximant theorem states when an approximant is expected to converge.

$\vdots$

- Jumps and Starts that invoke Baker & Gammel's idea, but nothing formalized as a method

$\vdots$

- 2012: (Barlow et al, J. Chem. Phys., 2012) An asymptotically consistent approximant for soft-sphere fluids
- 2013-2015: Additional papers in thermodynamics start to form a unified approach to solving problems where behavior is known at two ends.
- 2015-2017: Method, now coined "asymptotic approximants", applied to boundary layer problems in fluid dynamics. Leads to a methods Paper (Barlow et al, QJMAM, 2017).
- 2017-present: Nate and Steve start working with Josh as the method is applied to astrophysics. Leads to two papers on light bending and a collaboration with Ofek & CCRG folks on application to gravitational waves.

Example: Integral for light bending

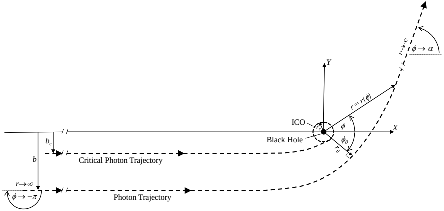
The governing equation for trajectories of light around a Kerr black-hole in the equatorial plane is given by

$$\phi(r) = \ll\pi + \int_0^{r_0/r} g(\hat{y}) d\hat{y}$$

where

$$g(\hat{y}) = \frac{u_0[b \ll 2u_0(b \ll a)\hat{y}]}{[1 \ll 2u_0\hat{y} + a^2u_0^2\hat{y}^2]\underline{\sum 1} + \hat{y} \ll 2(b \ll a)^2 u_0^3 \hat{y}^2\big)^{1/2}} \frac{d\hat{y}}{(1 \ll \hat{y})^{1/2}},$$

$u_0 = 1/r_0$, a is spin, and other parameters (b, r_0) defined below.



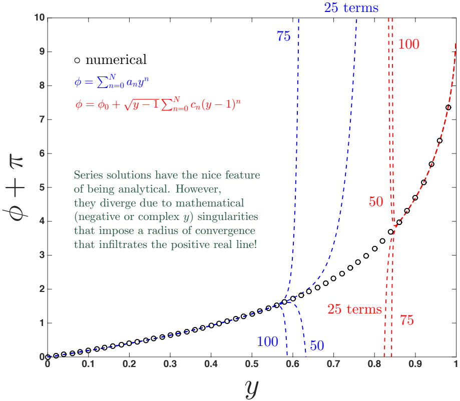
Chandrasekhar S 1983 *The mathematical theory of black holes, International Series of Monographs on Physics. Volume 69* (Clarendon Press/Oxford University Press).

Example: Integral for light bending

Let $y \equiv r_0/r$.

$$\phi(y) = \ll\pi + \int_0^y g(\hat{y})d\hat{y}$$

What can we do to solve this?



Solution shown here for $a = 1$, $b = 2.2222$.

Example: Integral for light bending

We can use the analytical information from the series, get past the radius of convergence, and bridge the gap in the solution as follows:

- We know that the expansion of the integral about $y = 0$ is

$$\phi = \sum_{n=0}^{\infty} a_n y^n$$

- We also know that the leading order behavior about $y = 1$ is

$$\phi = \phi_0 + c_0\sqrt{y \ll 1}$$

- Lets make up a function that (when expanded about $y = 0$) limits to the series above while also limiting to the square root behavior as $y \to 1$. How about this (bear with me here):

$$\phi_A = \phi_0 + \sqrt{1 \ll y}\sum_{n=0}^{\infty} A_n (y \ll 1)^n$$

- In this, we have already satisfied the correct leading $y \to 1$ behavior.
- The A_n are not known at this point! We will choose them in order to meet our other goal ...

Example: Integral for light bending

$$\phi_A = \phi_0 + \sqrt{1 \ll y} \sum_{n=0}^{\infty} A_n (y \ll 1)^n$$

We "choose" the A_n's such that the expansion of the above about $y = 0$ equals the expansion of the original integral about $y = 0$, namely:

$$\phi = \sum_{n=0}^{\infty} a_n y^n.$$

This can be viewed as solving a linear system (replace ∞ with N)

$$\phi_A(0) = f_0(A_0 \dots A_N) = a_0$$
$$\phi'_A(0) = f_1(A_0 \dots A_N) = a_1$$
$$\phi''_A(0) = f_2(A_0 \dots A_N) = 2\ a_2$$
$$\vdots$$
$$\phi_A^{(N)}(0) = f_N(A_0 \dots A_N) = N!\ a_N$$

But a matrix inversion is not saving us much (if any) over numerical integration of the original integral!! We can do better ...

Example: Integral for light bending

$$\phi_A = \phi_0 + \sqrt{1-y}\sum_{n=0}^{\infty} A_n (y-1)^n$$

1. Replace the LHS of above with expansion about $y = 0$

$$\sum_{n=0}^{\infty} a_n y^n = \phi_0 + \sqrt{1-y}\sum_{n=0}^{\infty} A_n (y-1)^n$$

2. Isolate the A_n series on one side

$$(1-y)^{-1/2}\left[-\phi_0 + \sum_{n=0}^{\infty} a_n y^n\right] = \sum_{n=0}^{\infty} A_n (y-1)^n$$

3. Expand the LHS of above about $y = 0$

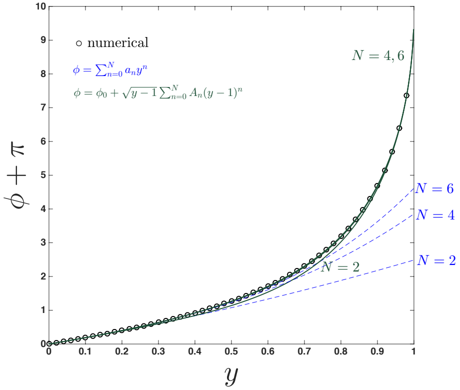
$$\sum_{n=0}^{\infty} G_n y^n = \sum_{n=0}^{\infty} A_n (y-1)^n$$

4. Replace ∞ with N and this becomes an identity with the solution for the coefficients

$$A_n = \frac{1}{n!}\sum_{m=0}^{N} \frac{\Gamma(m+1)}{\Gamma(m-n+1)} G_m$$

Example: Integral for light bending

The *Approximant* doesn't take that many terms before locking in!



Solution shown here for $a = 1$, $b = 2.2222$.

(show trajectory animation)

More details in:

R. J. Beachley, M. Mistysyn, J. A. Faber, S. J. Weinstein, and N. S. Barlow. Accurate closed-form trajectories of light around a kerr black hole using asymptotic approximants. Class. Quant. Grav., 35(20):128, 2018.

Obligatory Sherlock Holmes Quote

"See the value of imagination... We imagined what might have happened, acted upon the supposition, and found ourselves justified"

- A. C. Doyle from "Silver Blaze" (1892)

Asymptotic Approximants

- Hybrid of two well-known mathematical techniques
  - Asymptotic Matching - combining two *overlapping* asymptotic expansions
  - Padé Approximants - series expansion of rational function (polynomial over polynomial) about given point is same as true expansion about that point
- May be constructed when asymptotic behaviors are known in two different regions of a domain.
- Definition:
  - Form of approximant matches the behavior in one limit
  - Unknowns are chosen to match the behavior in the other limit

Definition (Barlow et al, QJMAM 2017)

Given a power series representation of some function $f(x)$:

$$f = \sum_{n=0}^{\infty} a_n (x - x_0)^n, \tag{1}$$

and an asymptotic behavior

$$f \to f_a(x) \text{ as } x \to x_a,$$

where $x_a \neq x_0$, an *asymptotic approximant* is any function $f_A(x)$ that may be expressed analytically in closed form and that satisfies the following three properties:

1. The N-term Taylor expansion of f_A about x_0 is identical to the N-term truncation of (1).
2. $\lim_{x \to x_a} (f_A/f_a) =$ constant for any N.
3. The sequence of approximants converges for increasing N.

Asymptotic approximants approximate and constrain the analytic continuation of an expansion such that the correct asymptotic limit (in some other region) is obtained.

Flow near a flat plate

steady, incompressible, 2-D, neglect gravity, $v \ll u$, $\frac{\partial}{\partial x} \ll \frac{\partial}{\partial y}$

governing "boundary layer" equations:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2}$$

boundary conditions:

$u = v = 0$ at $y = 0$
$u \to U$ as $y \to \infty$

Blasius (1908)
picture from Schlichting

or

$u = U$, $v = 0$ at $y = 0$
$u \to 0$ as $y \to \infty$

Sakiadis (1961)

Similarity transform

$$\eta = y\sqrt{U/(\nu x)},\ u = Uf'(\eta),\ v = [\eta f'(\eta) - f(\eta)]\sqrt{\nu U/(4x)}$$

single nonlinear ordinary differential equation in $f(\eta)$:

$$2f''' + ff'' = 0$$

boundary conditions:

Blasius Problem

$f(0) = f'(0) = 0,\ f'(\infty) \to 1$

Sakiadis Problem

$f(0) = 0,\ f'(0) = 1,\ f'(\infty) \to 0$

Power Series Solution to the Blasius/Sakiadis Problem

$$2f''' + ff'' = 0$$
$$f(0) = a_0,\ f'(0) = a_1,\ f'(\infty) \to b$$

$$f = \sum_{n=0}^{\infty} a_n x^n$$

$$a_{n+3} = \frac{-\sum\limits_{j=0}^{n} a_{n-j}(j+1)(j+2)a_{j+2}}{2(n+1)(n+2)(n+3)}.$$

- requires $f''(0) \equiv \kappa$, coefficient of the wall shear

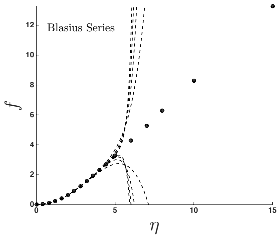
$$f = a_0 + a_1\eta + \frac{\kappa}{2}\eta^2 + a_3(\kappa)\eta^3 + a_4(\kappa)\eta^4 + \dots$$

- numerical estimates of κ:
  - Blasius flow: 0.33205733621519630 (Boyd, 1999)
  - Sakiadis flow: -0.44374733 (Cortell, 2010)

Power Series Solution to the Blasius/Sakiadis Problem

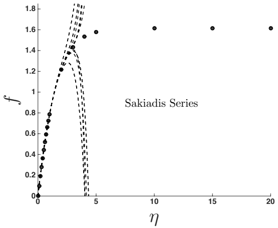
$$2f''' + ff'' = 0$$

Blasius Problem



$f(0) = f'(0) = 0,\ f'(\infty) \to 1$

Sakiadis Problem



$f(0) = 0,\ f'(0) = 1,\ f'(\infty) \to 0$

Approximant for the Blasius Problem

We start with an approximant form that matches $f\,'(\infty) \to 1$:

$$f_A = \eta + B \ll B \left(1 + \sum_{n=1}^{N} A_n \, \eta^n \right)^{-1}$$

and follow steps from before to find the A_n's:

1.
$$\sum_{n=0}^{\infty} a_n \eta^n = \eta + B \ll B \left(1 + \sum_{n=1}^{N} A_n \, \eta^n \right)^{-1}$$

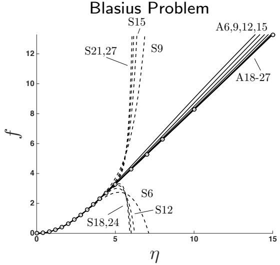
2.
$$\left[\eta / B + 1 \ll \frac{1}{B} \sum_{n=0}^{\infty} a_n \eta^n \right]^{-1} = 1 + \sum_{n=1}^{N} A_n \, \eta^n$$

3. Expand LHS about $\eta{=}0$. JCP Miller's formula leads to a recursive solution:

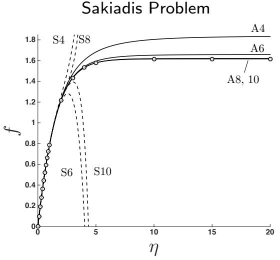
$$A_{n>0} = \frac{1}{B} \sum_{j=1}^{n} \tilde{a}_j \; A_{n-j}, \quad A_0 = 1, \quad \tilde{a}_1 = \ll 1, \quad \tilde{a}_{j>1} = a_j$$

Axproximants to the Blasius/Sakiadis Problem

$$2f''' + ff'' = 0$$



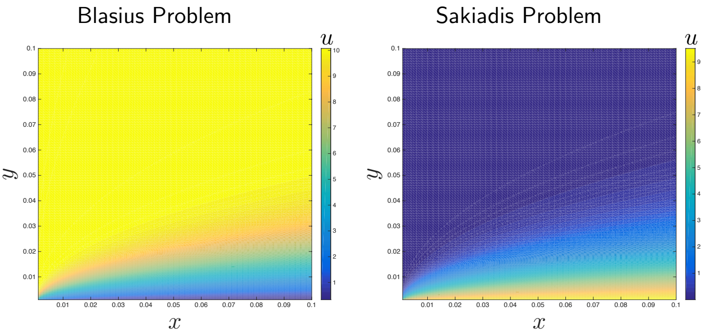
$f(0) = f'(0) = 0,\ f'(\infty) \to 1$



$f(0) = 0,\ f'(0) = 1,\ f'(\infty) \to 0$

(Barlow et al, QJMAM 2017)

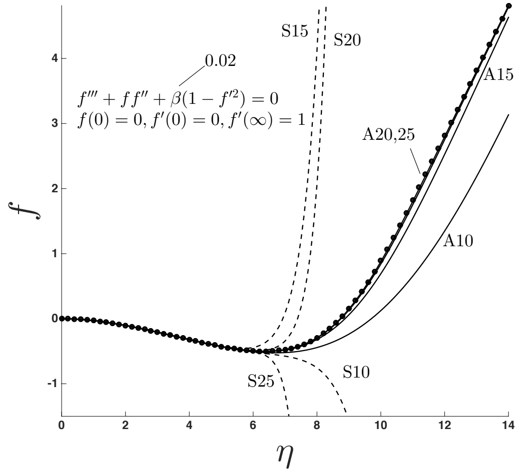
Transform back to physical variables



(Barlow et al, QJMAM 2017)

Some other nonlinear ODEs we've solved:

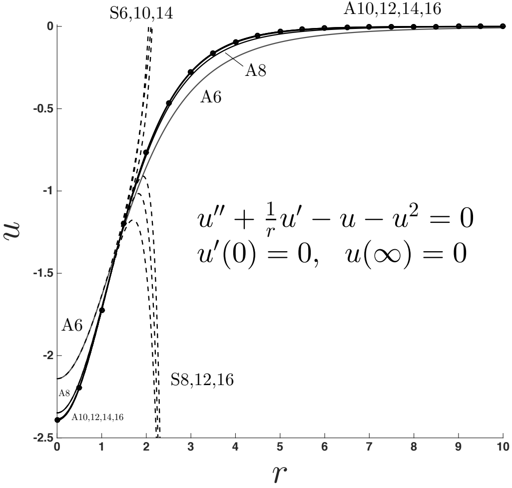
Falkner-Skan equation for boundary layers over a wedge



Belden et. al (to appear in QJMAM, Spring 2020)

Some other nonlinear ODEs we've solved:

Flieril-Petviashvili model for the motion of Jupiters red spot



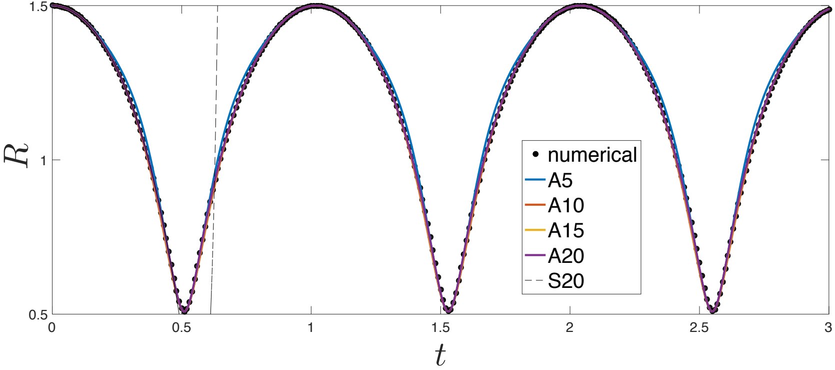
Barlow et. al. (QJMAM, 2017)

Some other nonlinear ODEs we've solved:

Currently Working on w/ A. Harkin, A. Giammarese, J. Tarantino:

Rayleigh-Plesset Equation for Oscillating Bubbles

$$R\ddot{R} + \frac{3}{2}(\dot{R})^2 + \delta\frac{1}{R} - \alpha\beta\frac{1}{R^3} = \gamma$$
$$R(0) = R_0,\ R'(0) = V_0$$



Let's try some harder problems...

What if you have no governing equation to start from (integral, differential equation, etc.) ?

What if you only have a **limited number of terms in an expansion**... and the expansion diverges?! (at some point)

This is the case for the **virial expansion** equation of state from thermodynamics.

$$\frac{P}{\rho kT} = 1 + B_2\rho + B_3\rho^2 + \ldots$$

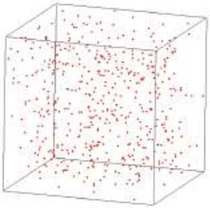
calculating fluid properties

Properties such as energy, entropy, etc. can be calculated by applying thermodynamic laws to an equation of state.

- ex. ideal gas

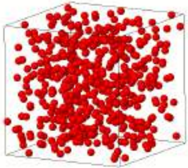
$$P = \rho k T$$

  - assumes no interaction b/w fluid molecules
  - valid when molecules are "far enough" apart (limit as $\rho \to 0$)



virial series

What if molecular interactions are important? (non-ideal fluid)



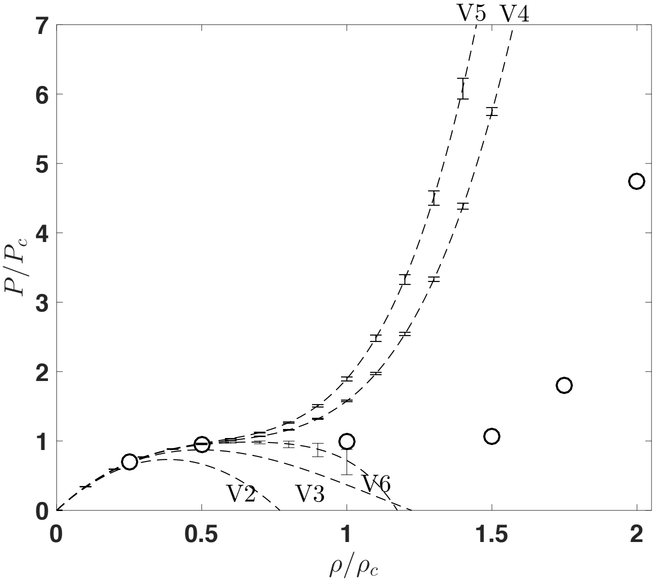
- virial equation of state (virial series)

$$P = kT \sum_{j=1}^{J} B_j(T)\rho^j$$

$$B_1 = 1, \quad B_2 = -\frac{1}{2}\int f_{1,2} d\mathbf{r}_{1,2}, \ldots B_8 = \text{18-dimensional integral}$$

  - intermolecular interactions accounted for
  - expansion of $P(\rho, T)$ about ρ=0 (ideal gas limit)

virial series for a model fluid (square-well)



critical point & scaling

- The thermodynamic critical point $(\rho, T, P) = (\rho_c, T_c, P_c)$ occurs where

$$\left(\frac{\partial P}{\partial \rho}\right)_{T,N} = 0; \ \left(\frac{\partial^2 P}{\partial \rho^2}\right)_{T,N} = 0; \ \left(\frac{\partial^3 P}{\partial \rho^3}\right)_{T,N} \geq 0.$$

- universal critical scaling:

$$(P - P_c)_{T_c} \sim C \ \mathrm{sgn}\left(1 - \frac{\rho}{\rho_c}\right)\left|1 - \frac{\rho}{\rho_c}\right|^{\delta} \quad \text{as} \quad \rho \to \rho_c$$

  - (Pelissetto & Vicari, *Phys Rep* 2002): $\delta = 4.789(2)$
  - branch-point singularity at $\rho = \rho_c$.

critical isotherm approximant

We start with an approximant form that matches scaling behavior:

$$P_A = P_c \ll \sum_{n=0}^{N} A_n \rho^n \left(1 \ll \frac{\rho}{\rho_c}\right)^{\delta}$$

and follow steps from before to find the A_n's:

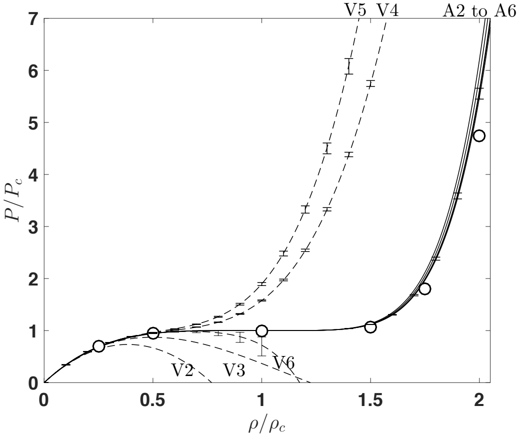
1. $$\left(P_c \ll kT_c \sum_{n=1}^{N} B_n(T_c)\rho^n\right)\left(1 \ll \frac{\rho}{\rho_c}\right)^{-\delta} = \sum_{n=0}^{N} A_n \rho^n$$

2. Expand LHS about ρ=0. JCP Miller's formula and Cauchy's product rule leads to a recursive solution:

$$A_n = \frac{P_c \Gamma(\delta + n)}{n! \rho_c^n \Gamma(\delta)} \ll \frac{kT_c}{\Gamma(\delta)} \sum_{j=0}^{n-1} \frac{B_{n-j}\Gamma(\delta + j)}{\rho_c^j \, j!}$$

critical isotherm approximant

$$P_A = P_c - \sum_{n=0}^{N} A_n \rho^n \left(1 - \frac{\rho}{\rho_c}\right)^{\delta}$$



(Barlow et al, JCP 2015)

Predict stuff from the approximant!

We have a critical isotherm approximant

$$P_A = P_c \ll \sum_{n=0}^{N} A_n \rho^n \left(1 \ll \frac{\rho}{\rho_c}\right)^{\delta}$$

with coefficients

$$A_n = \frac{P_c \Gamma(\delta + n)}{n! \rho_c^n \Gamma(\delta)} \ll \frac{kT_c}{\Gamma(\delta)} \sum_{j=0}^{n-1} \frac{B_{n-j}\Gamma(\delta + j)}{\rho_c^j \, j!}$$

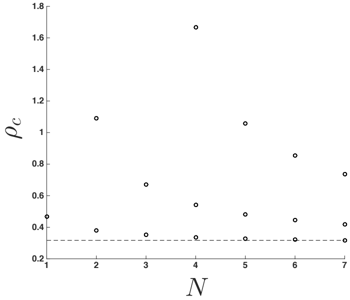
Recall that this could be posed as a system with N equations and N unknowns (A_0, A_1,. . . ,A_N). Lets swap an unknown. Let one of the inputs (ρ_c, P_c, δ) be an unknown, keep N equations, and let the series have one less coefficient. This is equivalent to letting A_N=0 in above, leading to

$$P_c \ll \frac{kT_c N!}{\Gamma(\delta + N)} \sum_{j=1}^{N} \frac{\Gamma(\delta + N \ll j)}{(N \ll j)!} B_j \rho_c^j = 0$$

The above can be used to predict P_c, ρ_c, or δ.

Predict stuff from the approximant!

$$P_c \ll \frac{kT_c N!}{\Gamma(\delta + N)} \sum_{j=1}^{N} \frac{\Gamma(\delta + N \ll j)}{(N \ll j)!} B_j \rho_c^j = 0$$



Given all other variables as inputs, the $\circ$'s are the fastest converging roots of the remaining ρ_c polynomial. The dashed line is the prediction from molecular simulations of a Lennard-Jones fluid.

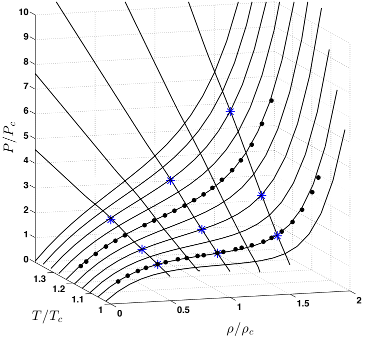
scaling $\rightarrow$ thermodynamic surface near c.p.

- along critical isotherm ($T = T_c$):

  $(P/P_c - 1) \sim \pm D_0 \; (1 - \rho/\rho_c)^{\delta}$

- along critical isochore ($\rho = \rho_c$):

  $\left(\frac{\partial P}{\partial \rho}\right)_{T>T_c} \sim 1/\Gamma^{+} \; (T/T_c - 1)^{\gamma}$

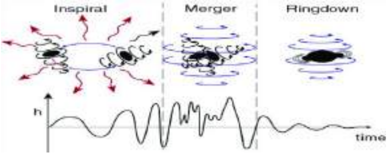


(Pelissetto & Vicari, 2002): $\delta = 4.789(2), \;\gamma = 1.2372(5)$

(Barlow et al, JCP 2015)

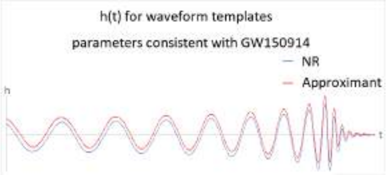
What's next on our plate?

Pre-2005 schematic:



K. S. Thorne, "Spacetime Warps and the Quantum World: Speculations about the Future," in R. H. Price, ed., The Future of Spacetime. W. W. Norton, New York, 2002, pp. 109-152.

Now thanks to Numerical Relativity:

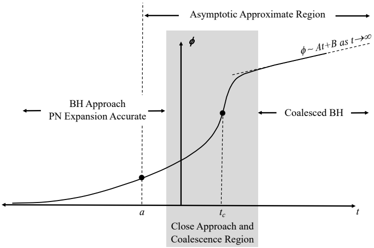


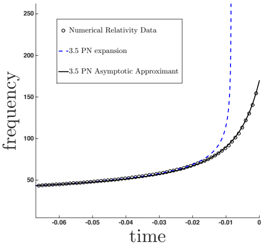
Taken from the Gravitational Wave Open Science Center

Gravitational Waveform Approximant

Preliminary Work:

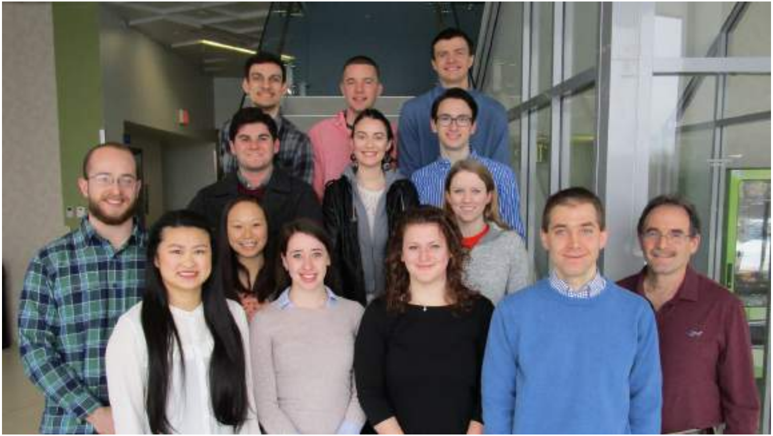
- Expand known PN expansion about some negative time $t = a$
- Ultimate Goal: Form approximant that matches this new expansion at $t = a$ and matches known behavior as $t \to \infty$, and hopefully (as in problems of the past) pick up everything in-between! (cartoon on left)
- Where we are now: constructed approximant that matches expansion at $t = a$ and inflection at $t = 0$. (figure on right)
- Joint NSF/BSF proposal submitted with Ofek Birnholtz . . . wish us luck!





On right: BHs of equal mass and zero spin. NR data in-house from Jam Sadiq.

Asymptotic Approximants Group



www.rit.edu/bwgroup

Asymptotic Approximants Group: References

Application to Astrophysics:

Beachley, Ryne J, Morgan Mistysyn, Joshua A Faber, Steven J Weinstein, and Nathaniel S Barlow. 2018. "Accurate Closed-Form Trajectories Of Light Around A Kerr Black Hole Using Asymptotic Approximants". Class. Quantum Grav. 35 (20)

Barlow, Nathaniel S, Steven J Weinstein, and Joshua A Faber. 2017. "An Asymptotically Consistent Approximant For The Equatorial Bending Angle Of Light Due To Kerr Black Holes". Class. Quantum Grav. 34 (135017)

Application to Thermodynamics:

Barlow, Nathaniel S, Andrew J Schultz, Steven J Weinstein, and David A Kofke. 2015. "Communication: Analytic Continuation Of The Virial Series Through The Critical Point Using Parametric Approximants". The Journal Of Chemical Physics 143 (071103).

Barlow, Nathaniel S, Andrew J Schultz, David A Kofke, and Steven J Weinstein. 2014. "Critical Isotherms From Virial Series Using Asymptotically Consistent Approximants". Aiche Journal 60l: 3336?3349.

Barlow, Nathaniel S, A. J Schultz, S. J Weinstein, and D. A Kofke. 2012. "An Asymptotically Consistent Approximant Method With Application To Soft- And Hard-Sphere Fluids". J. Chem. Phys. 137: 204102.

Application to Fluid Dynamics:

E. R. Belden, Z. A. Dickman, S. J. Weinstein, A. D. Archibee, E. Burroughs, and N. S. Barlow. 2020. "Asymptotic Approximant for the Falkner-Skan Boundary-Layer equation". Quarterly Journal Of Mechanics And Applied Mathematics. Accepted arxiv.org/abs/1907.09912

Barlow, Nathaniel S, Christopher R Stanton, Nicole Hill, Steven J Weinstein, and Allyssa G Cio. 2017. ?On The Summation Of Divergent, Truncated, And Underspecified Power Series Via Asymptotic Approximants?. Quarterly Journal Of Mechanics And Applied Mathematics 70 (1): 21-48.