Toward Rigorous Computation of Global Dynamics of Gradient PDEs

Jean-Philippe Lessard
Georgia Tech / Rutgers

Boca Raton - December 2006

We are interested in understanding the global dynamics of the Swift-Hohenberg PDE

$$
\text{(S-H)} \quad \begin{cases} u_t = (\nu - 1)u - 2u_{xx} - u_{xxxx} - u^3, \\[2em] u(\cdot, t) \in L^2[0, \frac{2\pi}{L_0}], \qquad \nu > 0, \\[1em] u(x,t) = u(x + \frac{2\pi}{L_0}, t), \qquad u(-x,t) = u(x,t). \end{cases}
$$

It is a gradient PDE and its energy is given by

$$
E(u) = \int_0^{\frac{2\pi}{L_0}} \left[\frac{1}{4}u^4 - \frac{\nu}{2}u^2 + \frac{1}{2}(1 + u_{xx})^2 \right] dx
$$

Since Swift-Hohenberg is a gradient PDE, the dynamics of interest consists of equilibria (steady state solutions) and connecting orbits between them.

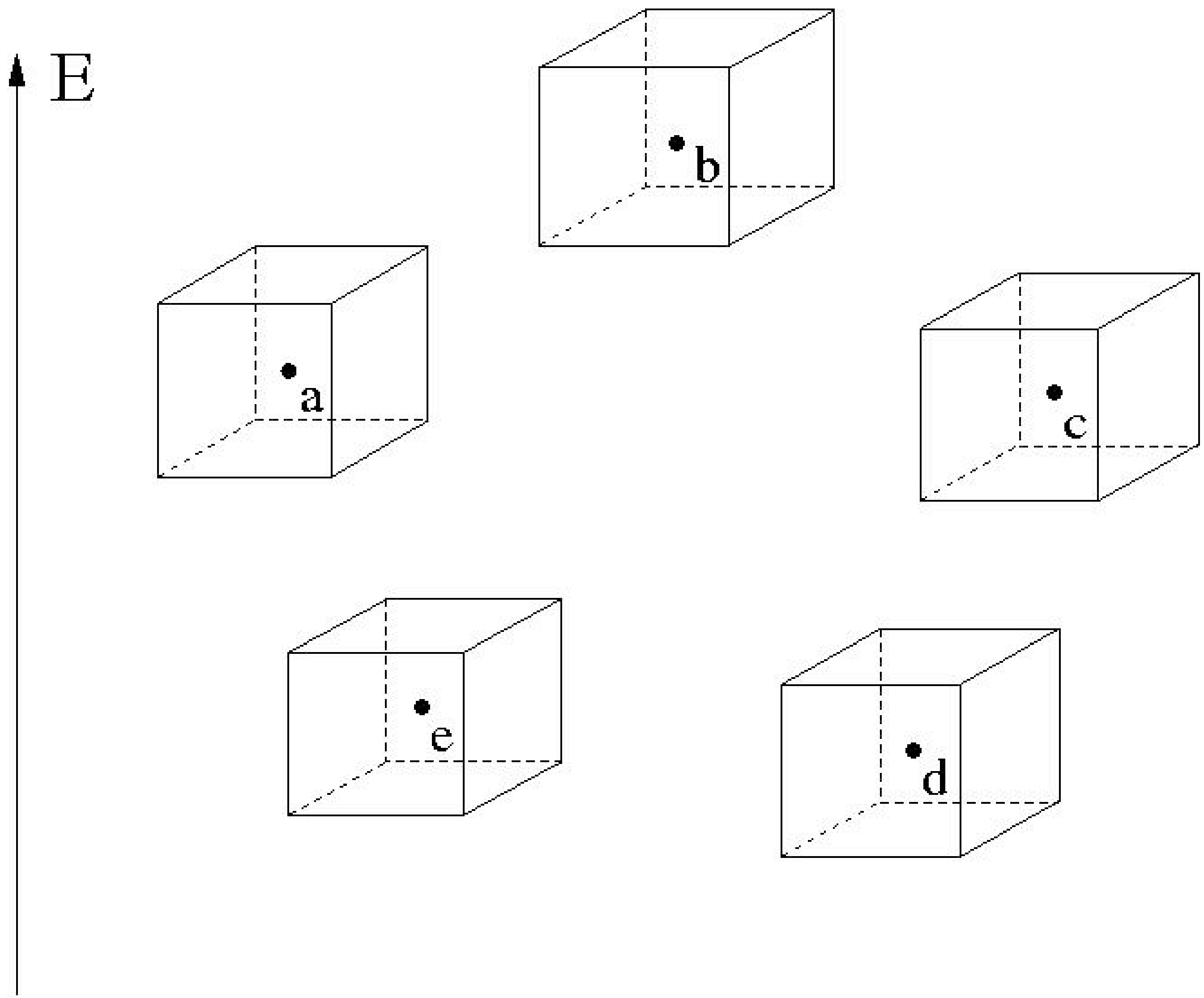
Connecting orbits are intersections of stable and unstable manifolds of equilibria. That raises the following question:

Is it possible to get rigorous approximations of the stable and unstable manifolds of equilibria of nonlinear PDEs ?

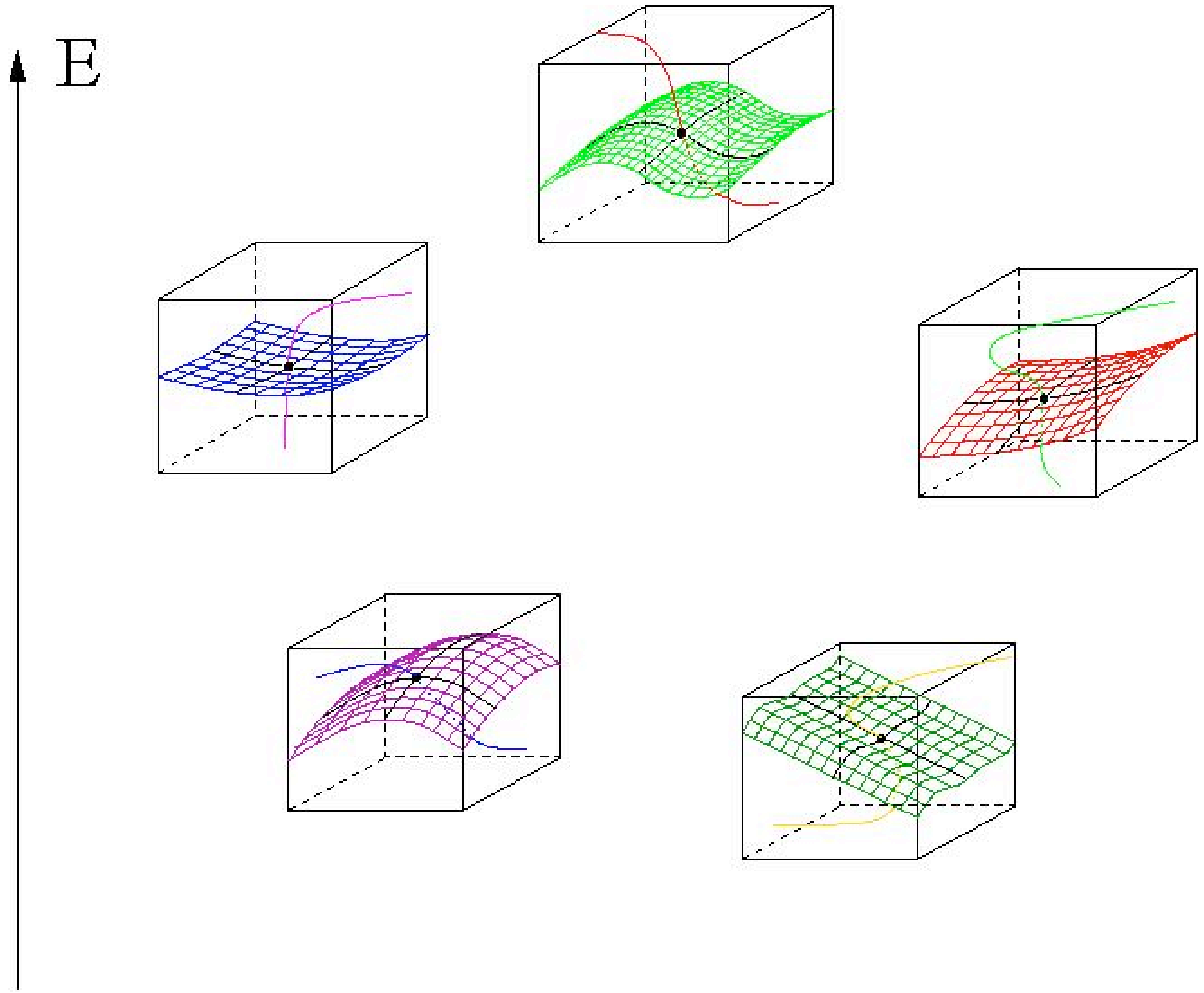
Outline in 4 parts

(1) Get a finite dimensional Galerkin projection of the original infinite dimensional PDE together with a priori analytic estimates of the truncation error term.

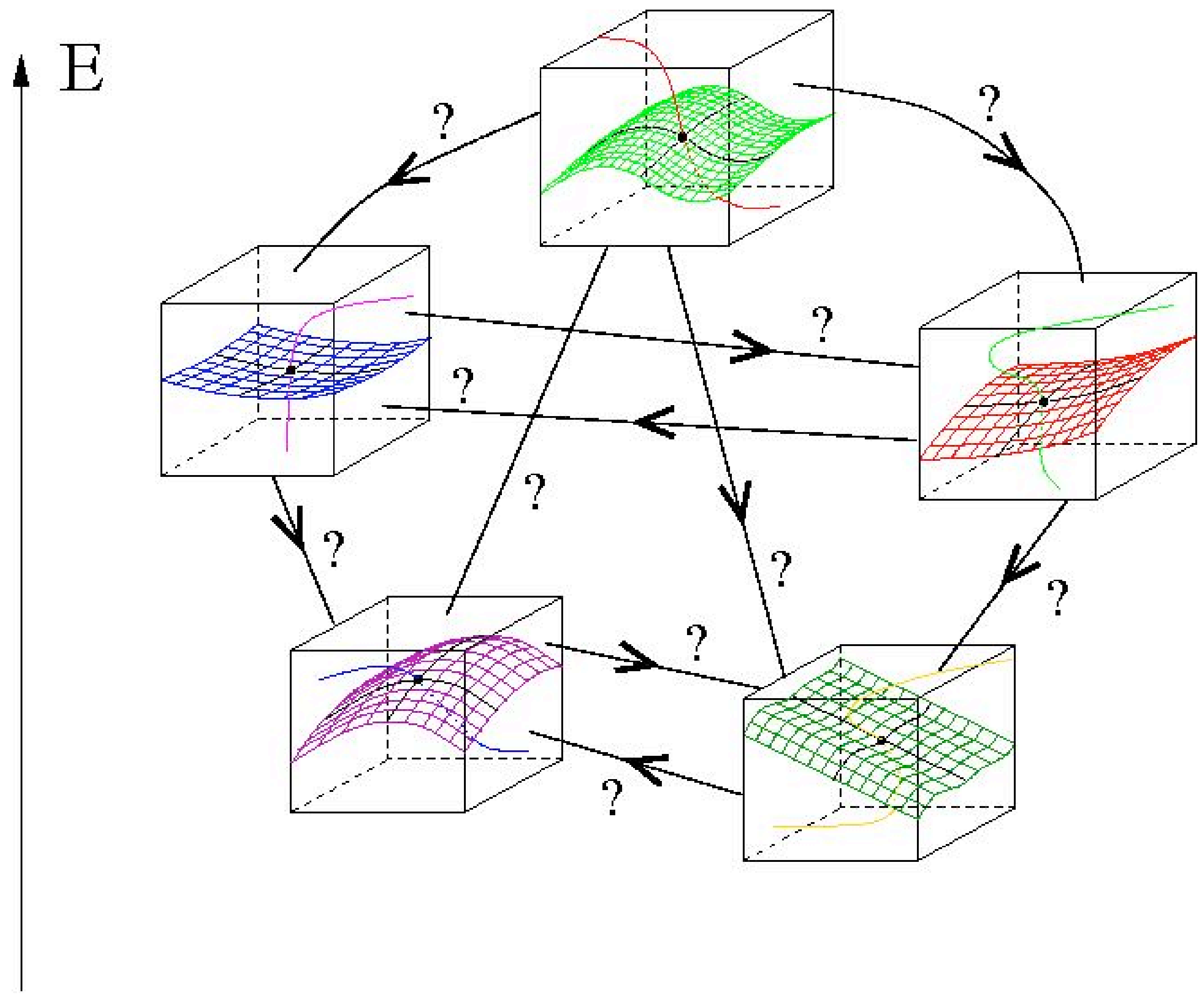
(2) Using a rigorous continuation method, we get small infinite dimensional sets containing a unique equilibrium of the original PDE: Validation Sets.



(3) We want representations of the stable and unstable manifolds of each of the equilibria of the PDE in each of the infinite dimensional validation sets.



(4) We want to determine the existence or nonexistence of connecting orbits between the validation sets.



(1) Galerkin Projection and Truncation Error Term

$$
\text{(S-H)} \quad \begin{cases} u_t = (\nu - 1)u - 2u_{xx} - u_{xxxx} - u^3, \\[2ex] u(\cdot, t) \in L^2[0, \frac{2\pi}{L_0}], \qquad \nu > 0, \\[1ex] u(x,t) = u(x + \frac{2\pi}{L_0}, t), \qquad u(-x,t) = u(x,t). \end{cases}
$$

Plugging $u(x,t) = \sum_{k=-\infty}^{\infty} c_k(t) e^{ikL_0 x}$ in (S-H), we get that

$$
\begin{aligned}
\sum_{k=-\infty}^{\infty} \dot{c}_k(t) e^{ikL_0 x} \quad = \quad & \sum_{k=-\infty}^{\infty} \left[(\nu - 1) + 2k^2 {L_0}^2 - k^4 {L_0}^4 \right] c_k(t) e^{ikL_0 x} \\
& - \left[\sum_{k_1=-\infty}^{\infty} c_{k_1}(t) e^{ik_1 L_0 x} \right] \left[\sum_{k_2=-\infty}^{\infty} c_{k_2}(t) e^{ik_2 L_0 x} \right] \left[\sum_{k_3=-\infty}^{\infty} c_{k_3}(t) e^{ik_3 L_0 x} \right]
\end{aligned}
$$

and taking the inner product in $L^2[0, \dfrac{2\pi}{L_0}]$ with each $e^{ikL_0 x}$:

$$
\dot{c}_k = \left[(\nu - 1) + k^2 L_0^2 - k^4 L_0^4 \right] c_k - \sum_{k_1 + k_2 + k_3 = k} c_{k_1} c_{k_2} c_{k_3} \ .
$$

Note that $u(x,t)$ being real implies that $c_{-k} = \overline{c_k}$ and that $u(-x,t) = u(x,t)$ implies that each c_k is real. Let $a_k = c_k$ such that $a_{-k} = a_k$. Define $a := (a_0, a_1, \cdots)$ and define

$$f_k(a) := \left[(\nu - 1) + k^2 L_0^2 - k^4 L_0^4\right] a_k - \sum_{k_1+k_2+k_3=k} a_{k_1} a_{k_2} a_{k_3} \ , \quad k \geq 0 \ .$$

Hence, we get the system of countably many ODEs

$$\dot{a}_k = f_k(a) \ , \quad k \geq 0$$

with corresponding finite dimensional Galerkin Projection

$$\dot{a}_k = f_k^{(m)}(a_F) := \left[(\nu - 1) + k^2 L_0^2 - k^4 L_0^4\right] a_k - \sum_{\substack{k_1+k_2+k_3=k \\ |k_1|,|k_2|,|k_3|<m}} a_{k_1} a_{k_2} a_{k_3} \ , \ k = 0, \cdots, m-1$$

where $a_F := (a_0, \cdots, a_{m-1})$ and $f^{(m)}(a_F) := [f_0(a_F, 0), \cdots, f_{m-1}(a_F, 0)]$.

The Truncation Error Term is defined by

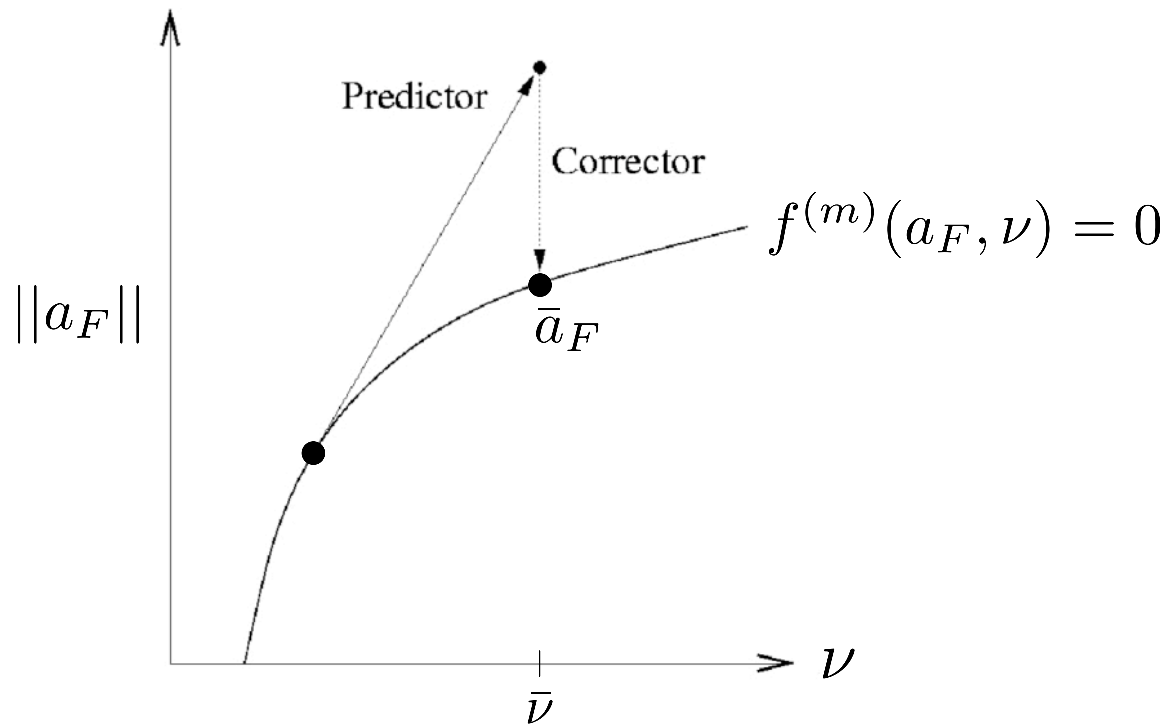
$$r_k(a) := \begin{cases} f_k(a) - f_k^{(m)}(a_F) \ , & \text{for } 0 \le k \le m-1 \\ f_k(a) \ , & \text{for } k \ge m \ . \end{cases}$$

For all k, suppose that $a_k \in \frac{A_s}{|k|^s}[-1,1]$ and let $\alpha := \frac{2}{s-1} + 2 + 3.5 \cdot 2^s$. Then for Swift-Hohenberg and for $0 \le k < m$, an a priori analytic estimate for the truncation error term is given by

$$\begin{aligned} r_k(a) &= - \sum_{\substack{k_1+k_2+k_3=k \\ \max\{|k_i|\} \ge m}} a_{k_1} a_{k_2} a_{k_3} \\ &\in \frac{2A_s^3}{m^{s-1}(s-1)} \left[\frac{1}{(m-k)^s} + \frac{1}{(m+k)^s} \right] [-1,1] \end{aligned}$$

(2) Rigorous Continuation for Equilibria of PDEs

To find the equilibria of $\dot{a} = f(a, \nu) = 0$, we use a recently developed rigorous continuation method based on a predictor-corrector algorithm.



Since the finite dimensional Newton-like map

$$T^{(m)}(a_F) := a_F - Df^{(m)}(\bar{a}_F)^{-1} f^{(m)}(a_F)$$

contracts small sets centered at the numerical equilibrium $\bar{a}_F$, we want to construct an infinite dimensional operator T that will contract small sets centered at $(\bar{a}_F, 0, 0, \cdots)$.

Let $\{ \mu_k := (\nu - 1) + k^2 L_0^2 - k^4 L_0^4 \mid k = 0, 1, \cdots\}$ the set of eigenvalues of the linear part $(\nu - 1) - 2\frac{\partial^2}{\partial x^2} - \frac{\partial^4}{\partial x^4}$ of Swift-Hohenberg and define

$$A := \begin{bmatrix} Df^{(m)}(\bar{a}_F)^{-1} & & 0 & \\ & \mu_m^{-1} & & \\ 0 & & \mu_{m+1}^{-1} & \\ & & & \ddots \end{bmatrix}.$$

Let's define the Newton-like operator $T(a) := a - Af(a)$.

For a projection dimension m large enough, we expect T to be close to the true Newton-like operator $N(a) := a - Df(\bar{a})^{-1} f(a)$ which should contract a small neighborhood of $\bar{a} = (\bar{a}_F, 0, 0, \cdots)$.

<u>New Goal</u>: Find $W_{\bar{a}}$ centered at $\bar{a}$ that will be contracted by T, where

$$\begin{aligned} W_{\bar{a}} &= \bar{a} + W(r) \\ &= \bar{a} + \prod_{k=0}^{m-1} [-r, r] \times \prod_{k=m}^{\infty} [-\frac{A_s}{k^s}, \frac{A_s}{k^s}] \, . \end{aligned}$$

For every $k \geq 0$, choose Y_k and Z_k such that

$$Y_k \geq |[T(\bar{a}) - \bar{a}]_k|$$

and

$$Z_k(r) \geq \sup_{w_1, w_2 \in W(r)} |[T'(w_1 + \bar{a})w_2]_k|$$

Theorem : Fix $s \geq 2$ and $A_s > 0$. If there exists an $r > 0$ such that

$$Y_k + Z_k(r) < r \ , \quad 0 \leq k < m$$

and that

$$Y_k + Z_k(r) < \frac{A_s}{k^s} \ , \quad k \geq m,$$

then T contracts $W_{\bar{a}}$. Such a set is called a *Validation Set.*

Let's fix $s \geq 2$ and $A_s > 0$. The *Finite Radii Polynomials* are defined by

$$p_k(r) = Y_k + Z_k(r) - r \ , \quad 0 \leq k < m$$

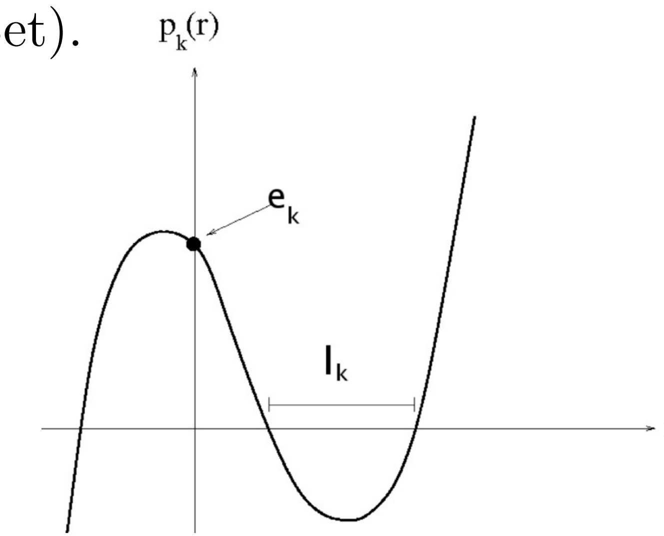
and the *Tail Radii Polynomials* are defined by

$$p_k(r) = Y_k + Z_k(r) - \frac{A_s}{k^s} \ , \quad k \geq m$$

Theorem: Let $s \geq 2$ and A_s fixed. If

$$\bar{r} \in \mathcal{I} := \bigcap_{k=0}^{\infty} \{ r > 0 \mid p_k(r) < 0 \} = [r_{\min}, r_{\max}]$$

then T contracts $W_{\bar{a}}(\bar{r})$ (which is then a Validation Set).



For Swift-Hohenberg, let $\nu = 1012.278335845298$, $m = 36$, $s = 2$ and $A_s = 1$. Then the first 5 radii polynomials are

$$P_0(r) = 3.78538693997847 r^3 + 53.66993812353729 r^2 - 0.94066816114817 r + 0.00002263158367$$

$$P_1(r) = 3.93318653216601 r^3 + 51.12414846239815 r^2 - 0.94501041465339 r + 0.00004390367633$$

$$P_2(r) = 4.34213973336531 r^3 + 43.70648160384567 r^2 - 0.95757138002609 r + 0.00009992391280$$

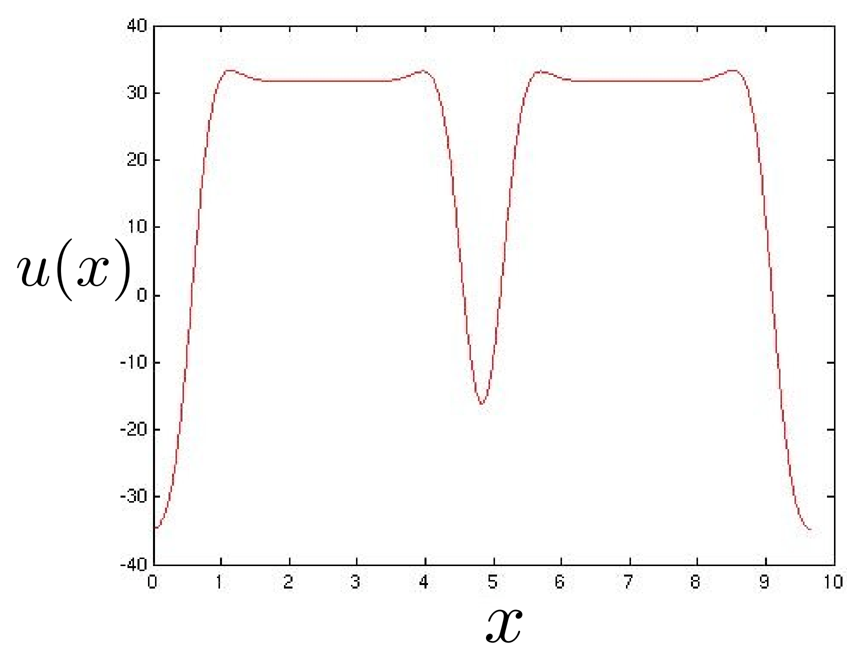
$$P_3(r) = 4.91217035583181 r^3 + 32.75454934434237 r^2 - 0.97595014905679 r + 0.00018439605102$$

$$P_4(r) = 5.48852159733388 r^3 + 19.85595518347044 r^2 - 0.99715843223739 r + 0.00027476033610$$

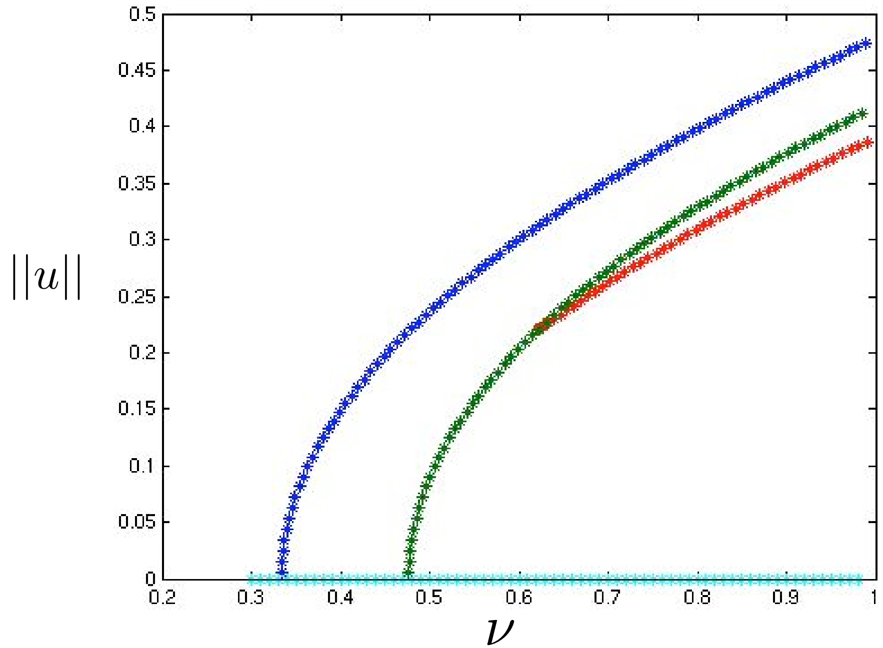
and $\mathcal{I} = [0.00042014834314 \; , \; 0.01748123404854]$

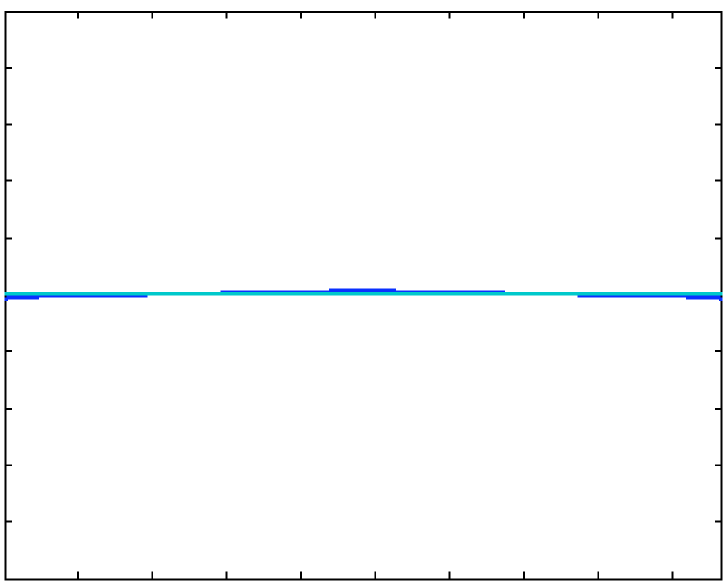
Theorem: Let $\nu = 1012.278335845298$, $s = 2$, $A_s = 1$ and $\bar{r} = 0.00042014834314$. Then the Swift-Hohenberg PDE has a unique equilibrium solution in the set

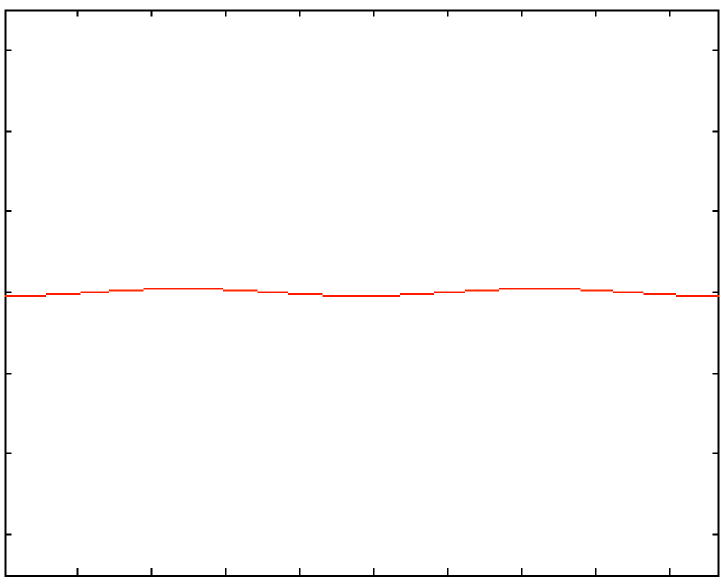
$$W_{\bar{a}} = (\bar{a}_F, 0, 0, \cdots) + \prod_{k=0}^{36} [-\bar{r}, \bar{r}] \times \prod_{k=37}^{\infty} \left[-\frac{1}{k^2}, \frac{1}{k^2} \right] .$$



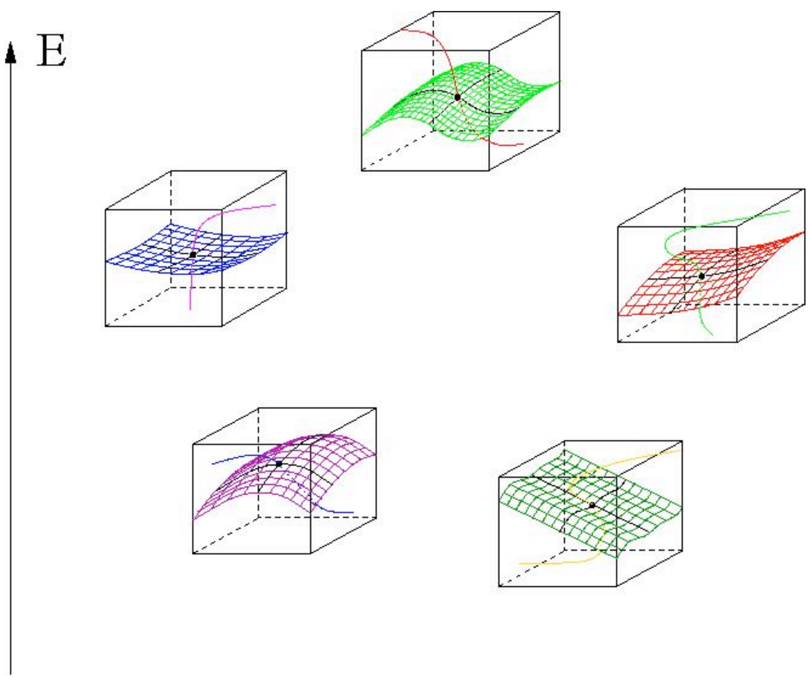
Using rigorous continuation, we obtained validation sets around each of the numerical equilibria shown in the picture below. These are equilibria for S-H.





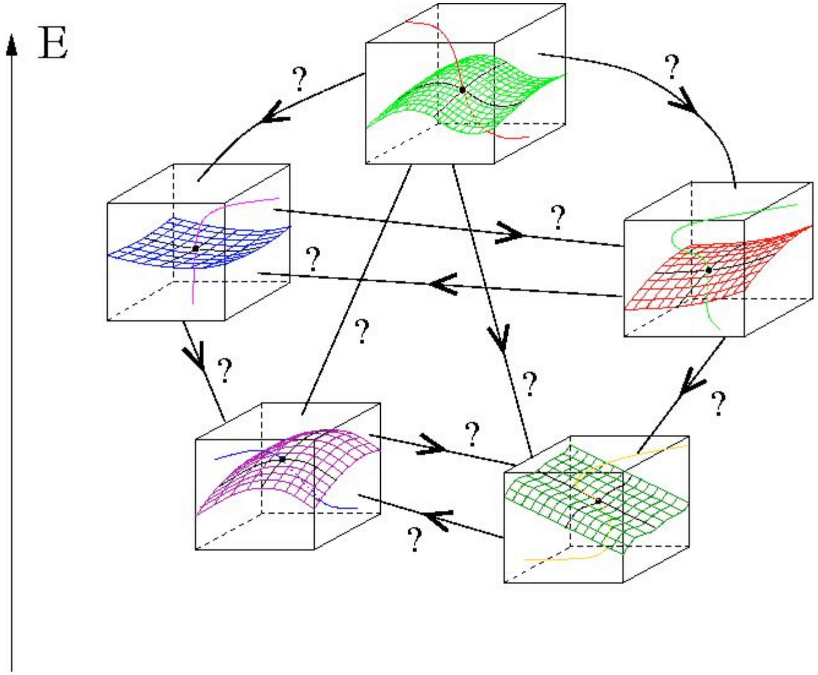


(3) Representations of the stable and unstable manifolds of each of the equilibria in their infinite dimensional validation sets using Taylor methods ?



- Analytic upper bounds of $f(\bar{a})$, $Df(\bar{a})$, $D^2 f(\bar{a})$, $D^3 f(\bar{a})$.

(4) Determine the existence or nonexistence of connecting orbits between the validation sets.



- Rigorous Integration using Taylor methods?
- Rule out connections using the energy.
- Think of a connecting orbit as a boundary value problem.

Work partially supported
by DARPA and DOE

Thank You !!