

Computer Assisted Proofs for Partial Differential Equations (SS 2012, KIT)

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16.04.2012

April 2012 --

- Lehrbeauftragte at KIT
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Nagatou or Nagato ???

長藤 かおり = な が と う か お り
na ga to u ka o ri

Pronunciation:
tou = to- (long "o")


Passport: Nagato Kaori

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CONTENTS


- Introduction
(Numerical Simulations and Reliable Computations)
- Basic concepts of Computer Assisted Proofs for PDEs
- Applications Lectures from next time

Introduction




17 pages

Basic idea




12 pages

Details



ϕ

Examples



22 pages

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Using a computer for Mathematics...

- 1) Numerical experiments
 - ➡ Numerical simulations, deriving a conjecture, ...
- 2) **Computer Assisted Proof**
 - ➡ Existence of solutions, uniqueness, ...

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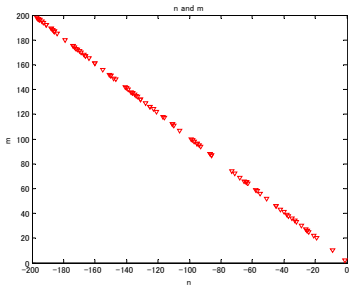
An example for 1)

For $x, y, z \in \mathbb{R}$ s.t. $x + y + z = 1, x < 0, 0 < y \notin \mathbb{Z}, z > 0$,
can we find integers m, n which satisfy

$$\frac{(m-1)x - y}{y+z} < n < \frac{mx + z}{y+z} \quad ?$$

➡ Numerical experiments

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We see a linear relation between m and n .
Moreover, m depends only on y .

➡ $m = \lfloor y \rfloor + 1, n = 1 - m$

Conjecture by a numerical experiment → Analytical proof

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Numerical Simulation

- How can we get an appropriate modeling for a phenomena?
- What is an appropriate mathematical formula for it?

Mathematical modeling for a numerical simulation

↓

We want to know how the phenomena changes.

Differential equations

↓

It is suitable to describe a variation.

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Our environment

↓

4 dim. (spatial 3-D [x, y, z] + time [t])

variation

space [changes on x, y, z]

time [changes on t]

One variable among x, y, z, t → ODE

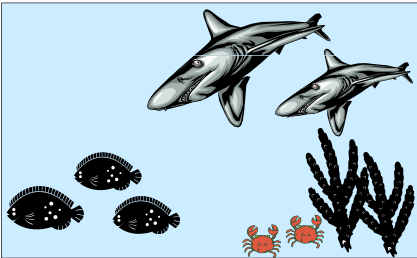
More than one variable among x, y, z, t → PDE

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Example of a numerical simulation: Predator-Pray problem

Pray → flatfish
Predator → shark

How does the number of flatfish and shark change depending on time?



The Adriatic Sea

The principle food of shark in this sea is flatfish.

There are enough foods for flatfish.

Flatfish does not fight against shark and is just eaten by shark.

American mathematician **Lotka** and Italian mathematician **Volterra** proposed a mathematical model for an interaction between shark and flatfish.

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$f(t)$: the number of flatfish at the time t
 $g(t)$: the number of shark at the time t

Assumption

- If there is no shark, then $f(t)$ increases as $f'(t) = af(t)$ ($a > 0$)
- If there is no flatfish, then $g(t)$ decreases as $g'(t) = -cg(t)$ ($c > 0$)
- Increasing rate of flatfish becomes small by shark: $-bg(t)$ ($b > 0$)
- Decreasing rate of shark becomes small by flatfish: $df(t)$ ($d > 0$)

Lotka – Volterra Model

Basic model for an interaction between two species.

There are many extended models, e.g. for predator-prey competition.

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Numerical "data" by solving the system of ODEs

($a = 0.01$, $b = d = 0.0001$, $c = 0.05$)

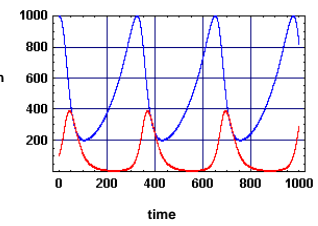
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0.4000000000000000	999.95973334948997	0.4000000000000000	102.020079311990096
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1.2000000000000000	999.63280399492396	1.2000000000000000	106.18210269406652
1.3000000000000000	999.56835180768746	1.3000000000000000	106.71391693121188
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1.7000000000000000	999.25705221791065	1.7000000000000000	108.86715472704331
1.8000000000000000	999.16573074523239	1.8000000000000000	109.41199127094350
1.9000000000000000	999.06896121156649	1.9000000000000000	109.95945109401094
2.0000000000000000	998.96671896548401	2.0000000000000000	110.50954025570091
⋮	⋮	⋮	⋮

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Visualization of these numerical data

Lotka – Volterra Model

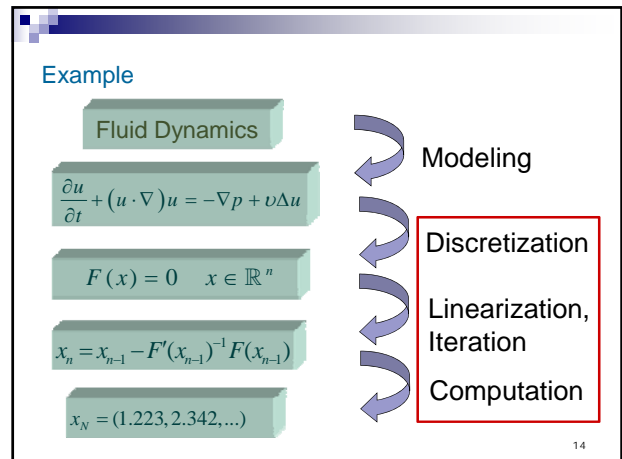
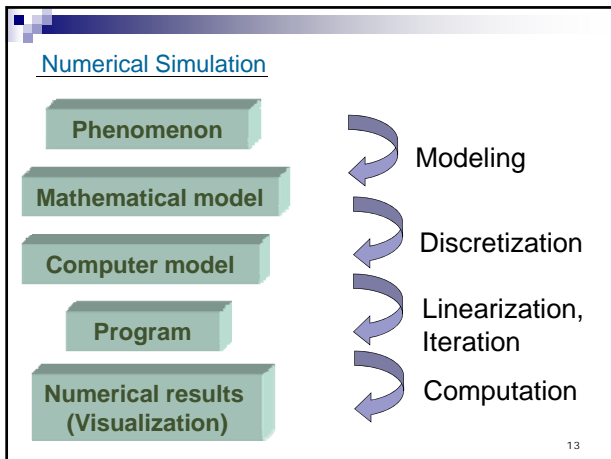
Initial values: $x(0)=1000$, $y(0)=100$



Blue: flatfish
Red: shark

time

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Available techniques to overcome rounding error problems by "reliable" arithmetic:

- Multiple Precision Arithmetic (GNU MP, OMNI, FMLIB, Mathematica, etc.)
- Rational Number Arithmetic (Mathematica, Maple, Reduce, etc.)

↓

More reliable, but not always exact & High cost

Interval Arithmetic (reliable with proof character)

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- Self-validating methods
 - Numerical verification
 - Computer-assisted proofs
 - Numerical computations with guaranteed accuracy
1. It guarantees the **existence** (and **local uniqueness**) of solutions
2. It guarantees **bounds** for the error between exact and approximate solution
3. All errors occurring in the numerical process are taken into account
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Basic tools

Interval Arithmetic & Fixed Point Formulation

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$X = [\underline{x}, \bar{x}], Y = [\underline{y}, \bar{y}] \subset \mathbb{R}$: intervals

$X * Y \equiv \{x * y \mid x \in X, y \in Y\}, \quad * \in \{+, -, \times, /\}$

$X + Y = [\underline{x} + \underline{y}, \bar{x} + \bar{y}]$

$X - Y = [\underline{x} - \bar{y}, \bar{x} - \underline{y}]$

$X \times Y = [\min\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}, \max\{\underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y}\}]$

$X / Y = X \times \left[\frac{1}{\bar{y}}, \frac{1}{\underline{y}} \right], \quad (0 \notin Y)$

e.g. $2/3 \times \sqrt{2} \in [0.6666, 0.6667] \times [1.414, 1.415]$
 $\subset [0.9425, 0.9434]$

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Interval Arithmetic Software

INTLAB	Matlab toolbox
PROFIL	C++ class library
INTLIB	Fortran 90 module
Sun ONE Studio	Interval operation on Fortran 95 and C++
<i>Mathematica</i>	Interval

```
e.g. INTERVAL X(1,2), Y(3.14,3.15);
cout << X*Y;
```

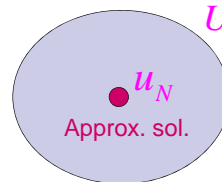
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Fixed Point Theorem

$$F(U) \subset U \Rightarrow \exists u \in U \text{ s.t. } u = F(u)$$

$$\left[F(U) = \{F(u) \mid u \in U\} \right]$$

Brower, Schauder, Banach etc.



Existence of a solution
Error between the exact solution and the approximate solution

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Basic concepts of Computer Assisted Proofs for Nonlinear PDEs

Methods based on functional analysis, especially on fixed point theorems in Sobolev spaces

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Transformation to a fixed point equation

Solve $-\Delta u = f(u)$



Find $u \in X$ satisfying $u = T(u)$ [Fixed Point Equation]

e.g. ω : An approximate solution

Infinite dimensional Newton's method

$$u = u - [-\Delta - f'(\omega)]^{-1} (-\Delta u - f(u)) =: T(u)$$



We need to estimate L^{-1} for the linearized operator $L \equiv -\Delta - f'(\omega)$

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Estimation of L^{-1}

Based on eigenvalues

L : self-adjoint

$$\lambda_* \in \sigma(L) \text{ (with the smallest absolute value)} \longrightarrow \|L^{-1}\| \leq \frac{1}{|\lambda_*|}$$

L : non self-adjoint

$$\mu_* \in \sigma(L^*L) \text{ (with the smallest absolute value)} \longrightarrow \|L^{-1}\| \leq \frac{1}{\sqrt{|\mu_*|}}$$

possibly combined with embeddings and a priori bounds

$$\|u\| \leq \kappa \|Lu\|$$

Based on the equation $Lu = 0$

Prove that $Lu = 0$ has the unique solution $u \equiv 0$ and estimate L^{-1} by additional computer assisted means ²³

[Plum]

Find u s.t. $\mathcal{F}(u) = -\Delta u - f(u) = 0$, $\mathcal{F}: X \rightarrow Y$,

$\omega \in X$: approximate solution $L = \mathcal{F}'(\omega): X \rightarrow Y$

$$\|\mathcal{F}(\omega)\|_Y \leq \delta$$

$$\|u\|_X \leq K \|Lu\|_Y \text{ for all } u \in X \quad \text{Eigenvalue Problem}$$

$$\|\mathcal{F}'(\omega + u) - \mathcal{F}'(\omega)\|_{B(X,Y)} \leq g(\|u\|_X) \text{ for all } u \in X$$

$$\left[g(t) \rightarrow 0 \text{ (} t \rightarrow 0 \text{)} \right]$$

$$\delta \leq \frac{\alpha}{K} - \int_0^\alpha g(t) dt \text{ for some } \alpha > 0$$

$$\Rightarrow \exists u \in X : \text{solution of } \mathcal{F}(u) = 0 \text{ s.t. } \|u - \omega\|_X \leq \alpha$$

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[Nakao]

Find $u \in X$ satisfying $-\Delta u = f(u)$



Find $u \in X$ satisfying $u = F(u)$ **【Fixed Point Equation】**



$P_h : X \rightarrow X_h$ (finite dimensional subspace of X)

$\begin{cases} P_h u = P_h F(u) & \dots \text{Newton's method with interval coefficients} \\ (I - P_h)u = (I - P_h)F(u) & \dots \text{Estimation by norm} \end{cases}$ **Linear system**

Error estimation for P_h is needed with an **explicit** constant

e.g. $\|v - P_h v\|_X \leq Ch \|\Delta v\|_V$

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Eigenvalue Enclosing method

L : self-adjoint operator

For simplicity, assume that a complete orthonormal system of eigenfunctions exists

Krylov-Weinstein's bound (1935)

$(\tilde{u}, \tilde{\lambda}) \in D(L) \times \mathbb{R}$ **approximate eigenpair**

$\delta \equiv \|L\tilde{u} - \tilde{\lambda}\tilde{u}\| / \|\tilde{u}\|$

\Rightarrow The interval $[\tilde{\lambda} - \delta, \tilde{\lambda} + \delta]$ contains at least one eigenvalue of L

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Kato's bound (1949)

$\tilde{u} \in D(L) \setminus \{0\}, \tilde{\lambda} \equiv \langle L\tilde{u}, \tilde{u} \rangle / \langle \tilde{u}, \tilde{u} \rangle$

$\delta \equiv \|L\tilde{u} - \tilde{\lambda}\tilde{u}\| / \|\tilde{u}\|$

For some $n \in \mathbb{N}$

$\min \{ \lambda_{n+1} - \tilde{\lambda}, \tilde{\lambda} - \lambda_{n-1} \} \geq \mu > 0 \quad (\lambda_0 \equiv -\infty)$

$\Rightarrow \lambda_n \in \left[\tilde{\lambda} - \frac{\delta^2}{\mu}, \tilde{\lambda} + \frac{\delta^2}{\mu} \right]$

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Rayleigh-Ritz method

$\tilde{u}_1, \dots, \tilde{u}_N \in D(L)$: linearly independent trial functions

$A_1 \equiv \left(\langle L\tilde{u}_i, \tilde{u}_j \rangle \right)_{i,j=1,\dots,N}, \quad A_2 \equiv \left(\langle \tilde{u}_i, \tilde{u}_j \rangle \right)_{i,j=1,\dots,N}$

$A_1 x = \Lambda A_2 x, \quad x \in \mathbb{R}^N \setminus \{0\}$

$\Rightarrow \lambda_n \leq \Lambda_n \quad (n = 1, \dots, N)$

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(Right-definite) Lehmann method (1963)

$\tilde{u}_1, \dots, \tilde{u}_N \in D(L)$: linearly independent trial functions

For some $\nu \in \mathbb{R}$ **s.t.** $\Lambda_N < \nu \leq \lambda_{N+1}$

$A_3 \equiv \left(\langle L\tilde{u}_i, L\tilde{u}_j \rangle \right)_{i,j=1,\dots,N}$

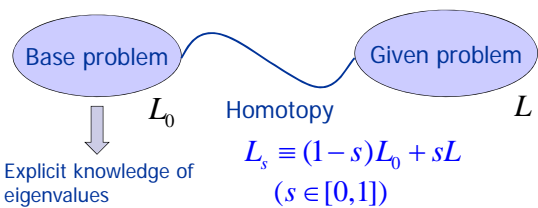
$B_1 \equiv A_1 - \nu A_2, \quad B_2 \equiv A_3 - 2\nu A_1 + \nu^2 A_2$

$B_1 x = \mu B_2 x$

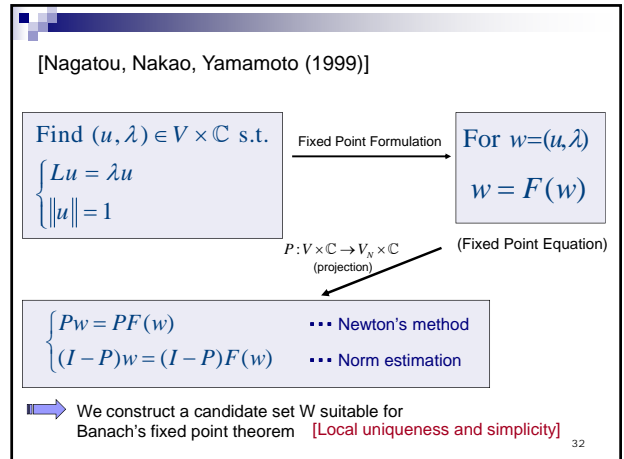
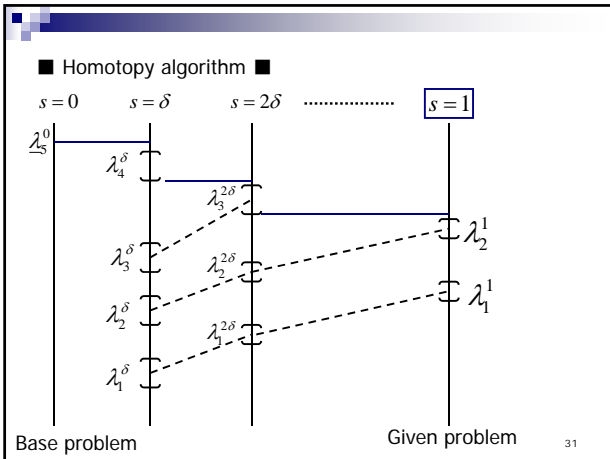
$\Rightarrow \lambda_{N+1-n} \geq \nu + \frac{1}{\mu_n} \quad (n = 1, \dots, N)$

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Homotopy method (Plum 1990)



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Applications

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Ex. 1: Allen-Cahn equation [Watanabe, Nakao (1993)]

(1)
$$\begin{cases} -\Delta u = \lambda u(u - a)(1 - u) & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

$\lambda = 150, a = 0.01, \Omega = (0,1) \times (0,1)$

ϕ_j : piecewise bilinear polynomials

The interval $(0,1)$ was partitioned into 80 pieces

Approx. sol.
(upper branch)

y=0.5

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Ex.2: Gelfand equation [Plum, Womersley (2002)]

(2)
$$\begin{cases} -\Delta u = \lambda e^u & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

$\lambda = 15/32$

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Ex.3: Computational multiplicity proof [Breuer, McKenna, Plum (2003)]

(3)
$$\begin{cases} \Delta u + u^2 = s \cdot \sin(\pi x_1) \sin(\pi x_2) & \text{in } \Omega = (0,1) \times (0,1) \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

It had been conjectured in the PDE community since the 1980's that Problem (3) has at least 4 solutions for $s > 0$ sufficiently large.

Computer assisted proof for $s = 800$

cf. Dancer & Yan (2005)

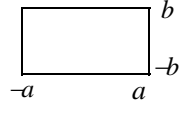
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Ex. 4: Linearized eigenvalue problem for Kolmogorov Problem [Nagatou (2004)]

Navier-Stokes equations:

$$(4) \begin{cases} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \frac{1}{R} \Delta u - \frac{1}{\rho} \frac{\partial p}{\partial x} + \gamma \sin\left(\frac{\pi y}{b}\right) \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = \frac{1}{R} \Delta v - \frac{1}{\rho} \frac{\partial p}{\partial y} \\ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \end{cases}$$

Flow region: periodic B.C



We wish to investigate the stability of solutions bifurcating from the basic flow

$$(u, v, p) = \left(c \sin\left(\frac{\pi y}{b}\right), 0, d \right) \quad \left(0 < \frac{b}{a} < 1 \right)$$

with the Reynolds number as a bifurcation parameter.



Linearized Eigenvalue Problem **Non-selfadjoint**

(Especially we need a basis of the nullspace of the linearized operator)

The first bifurcation point is: $(b/a = 0.7)$

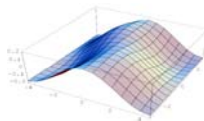
$$R \in [3.011528364444, 3.011528364446]$$

eigenfunction (ϕ_1)

- Maximum width of the interval for enclosing of the finite part:

$$3.000636 \times 10^{-14}$$

- Error: $|\tilde{\phi}_1 - P_N \tilde{\phi}_1|_{H^3(\Omega_x)} \leq 9.168914 \times 10^{-10}$



We enclosed the crucial eigenpair for the linearized operator and its adjoint operator. Using those eigenfunctions, we can decide if the bifurcating solution is stable or not.

Ex.5: Travelling waves in a nonlinearly supported beam

[Breuer, Horak, McKenna, Plum (2006)]

$$u_{tt} + u_{xxxx} + e^u - 1 = 0, \quad (x, t) \in \mathbb{R} \times \mathbb{R}^+$$



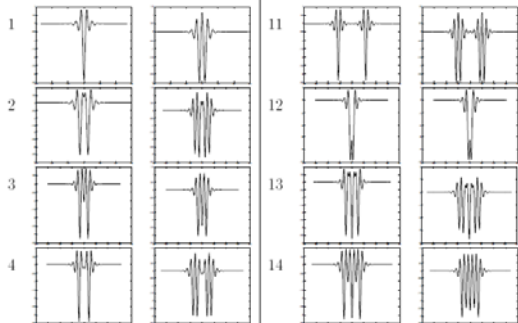
Solitary waves $u = \varphi(x + ct)$

$$\varphi^{iv} + c^2 \varphi'' + e^\varphi - 1 = 0 \quad (5)$$

Theorem:

For $c = 1.3$, Eq. (5) has at least 36 solutions.

lower branch upper branch # lower branch upper branch

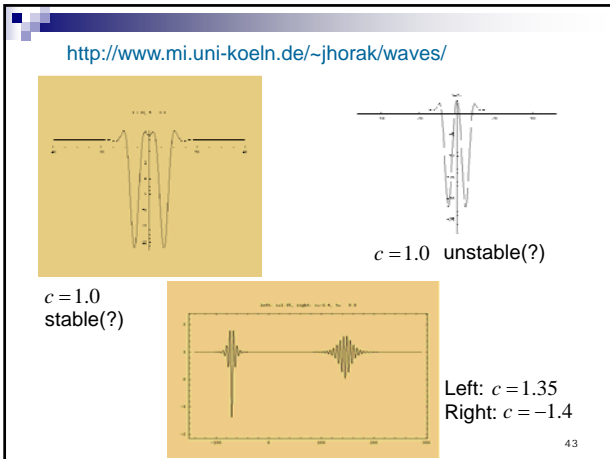


[Breuer, Horak, McKenna, Plum (2006)]

Open questions:

- Does at least one (or more than one) solution exist for all $c \in (0, \sqrt{2})$?
- Can one prove that as $c \rightarrow 0$, the number of solutions goes to infinity?
- Are the enclosed solutions stable or unstable?
- Is there any connection between the Morse index of a solution and its other properties, such as for example, its shape?

etc.



Theoretical results by Grillakis et al.

M. Grillakis, J. Shatah, W. Strauss
Stability Theory of Solitary Waves in the Presence of Symmetry, I & II (1986, 1989)

Abstract Hamiltonian system:

$$\frac{du}{dt} = JE'(u(t)) \quad (6)$$

- Locally well-posed in a space X
- E is a functional (the "energy")
- J is a skew-symmetric linear operator

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Assumption

Eq. (6) is invariant under an action $T(\cdot)$ of a group G on X .

$G = (\mathbb{R}, +)$
 $u(t) = T(ct)\varphi$,
 where $\varphi = \varphi_c$ depends on $c \in \mathbb{R}$. Solitary waves, Bound states

$\{T(g)\varphi : g \in G\}$ φ -orbit

φ -orbit is **stable**

$\stackrel{\text{def}}{\Leftrightarrow}$ a solution $u(t)$ of (6) exists for all $t \geq 0$ and forever remains near the φ -orbit (in the norm of X) provided that its initial datum $u(0)$ is sufficiently close to φ (in the norm of X).

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Q : another conserved functional (the "charge")
 (The vector φ is a critical point of $E - cQ$.)

$H_c := E''(\varphi_c) - cQ''(\varphi_c)$ linear operator
 $d(c) := E(\varphi_c) - cQ(\varphi_c)$ scalar function

$n(H)$: The number of negative eigenvalues of H_c

Stability/Instability Theorem [Grillakis et al. (1990)]

$d''(c) > 0, n(H_c) = 1 \Rightarrow \varphi$ -orbit is **stable**
 $d''(c) < 0, n(H_c) : \text{odd} \Rightarrow \varphi$ -orbit is **unstable**

(In case of $G = (\mathbb{R}, +)$)

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$u_t + u_{xxxx} + f(u) = 0, (x, t) \in \mathbb{R} \times \mathbb{R}^+$ ($f(u) = e^u - 1$)
 $X := H^2(\mathbb{R}) \times L^2(\mathbb{R}), X' = H^{-2}(\mathbb{R}) \times L^2(\mathbb{R})$
 $G = (\mathbb{R}, +), (T(g)[\phi])(x) = \phi(x + g)$

$v := u_t, U(t) := \begin{pmatrix} u \\ v \end{pmatrix} (c, t) \in X$

$\rightarrow U'(t) = \begin{pmatrix} u_t \\ u_{tt} \end{pmatrix} (c, t) = \begin{pmatrix} v \\ -u_{xxxx} - f(u) \end{pmatrix} (c, t) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} u_{xxxx} + f(u) \\ v \end{pmatrix} (c, t)$

$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} : H^{-2}(\mathbb{R}) \times L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}) \times H^{-2}(\mathbb{R})$

$E \left(\begin{pmatrix} u \\ v \end{pmatrix} \right) := \int_{\mathbb{R}} \left(\frac{1}{2} v^2 + \frac{1}{2} u_{xx}^2 + F(u) \right) dx, F' = f$

$Q \left(\begin{pmatrix} u \\ v \end{pmatrix} \right) := \int_{\mathbb{R}} u_x v dx$

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Ex. 6: Spectrum of a 1-D Schroedinger operator
[Nagatou, Plum, Nakao (2011)]

We consider the following eigenvalue problem:

(7) $-u'' + q(x)u + s(x)u = \lambda u, x \in \mathbb{R}$

$\left[\begin{array}{l} q : \text{bounded, continuous, periodic} \\ s \in L^\infty(\mathbb{R}), s(x) \rightarrow 0 \text{ as } x \rightarrow \pm\infty \end{array} \right]$

Non-existence proof of point spectrum in a spectral gap

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Eigenvalue Excluding Method

Let Λ be a sufficiently narrow interval and consider a linear equation

$$(L - \Lambda)u = 0 \quad \text{on } \mathbb{R} \quad (8)$$

Since it is clear that (8) has the trivial solution $u \equiv 0$, if we could validate the **uniqueness** of the solution of (8) by the method described below then it implies that any $\lambda \in \Lambda$ is NOT an eigenvalue of L , i.e. there is no eigenvalue in Λ .

Computer assisted proof for the uniqueness of solution for (8)

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Uniqueness of the solution for $-u'' + q(x)u + s(x)u - \lambda u = 0$

↑
Uniqueness of the solution for $u = F_\lambda(u)$

$$\left\{ \begin{aligned} F_\lambda(u) &= \int_{\mathbb{R}} G(x, y, \lambda) s(y) u(y) dy \\ G(x, y, \lambda) &= \begin{cases} \psi_1(x) \psi_2(y) & (x \leq y) \\ \psi_2(x) \psi_1(y) & (x \geq y) \end{cases} \end{aligned} \right.$$

↑
Fundamental solutions ψ_1, ψ_2 of $-\psi'' + q(x)\psi - \lambda\psi = 0$

↑
 ϕ_1, ϕ_2 in $[0, r]$ $\left\{ \begin{aligned} \phi_1(0) &= 1, \quad \phi_1'(0) = 0 \\ \phi_2(0) &= 0, \quad \phi_2'(0) = 1 \end{aligned} \right.$

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$$q(x) = a \cdot \cos(2\pi x), \quad s(x) = c \cdot e^{-x^2}$$

The interval Λ was subdivided into narrow subintervals Λ_k whose widths are 0.001 ~ 0.01.

Eigenvalue-free intervals

	Λ	The first spectral gap
$a = 3, c = 1$	[8.822, 10.585]	[8.341644, 11.340563]
$a = 3, c = 2$	[9.0, 9.35]	[8.341644, 11.340563]
$a = 5, c = 1$	[7.55, 11.335]	[7.292924, 12.287917]

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Ex. 7: 3-D Rayleigh-Bénard Problem

[Kim, Nakao, Watanabe, Nishida (2009)]

Oberbeck-Boussinesq equations

$$\left\{ \begin{aligned} \frac{1}{\text{Pr}} \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] + \nabla p &= \Delta \mathbf{u} - (G - \text{Ra } T) \mathbf{e}_z \\ \nabla \cdot \mathbf{u} &= 0 \\ \frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T &= \Delta T \end{aligned} \right.$$

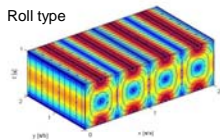
\mathbf{u} = velocity field
 p = pressure
 T = temperature
 Ra = Rayleigh number
 Pr = Prandtl number
 G = parameter

$$\Omega = \left\{ 0 \leq x \leq \frac{2\pi}{a}, \quad 0 \leq y \leq \frac{2\pi}{b}, \quad 0 \leq z \leq \pi \right\}$$

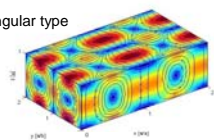
Obvious equilibrium $\mathbf{u}=0$, T : linear, p : quadratic in z . They investigated bifurcations from this static solution with Ra as a bifurcation parameter.

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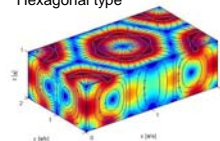
Roll type



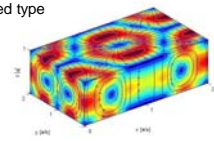
Rectangular type



Hexagonal type



Mixed type

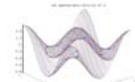
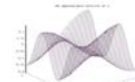
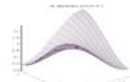


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Ex. 8: Reaction-Diffusion equations (2D, Neumann B.Cs)

[Cai, Nagatou, Watanabe (2012)]

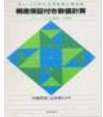
$$\left\{ \begin{aligned} \frac{\partial u}{\partial t} &= D_u \Delta u + f(u, v) \\ \frac{\partial v}{\partial t} &= D_v \Delta v + g(u, v) \end{aligned} \right. \quad \begin{aligned} f(u, v) &= u - u^3 - \delta v \\ g(u, v) &= \varepsilon(u - \gamma v) \end{aligned}$$



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References

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Existence and Multiplicity Proofs for Semilinear Elliptic Boundary Value Problems by Computer Assistance. DMV Jahresbericht: JB 110, Band (2008), Heft 1, 19-54.
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Computer-assisted Proofs for Semilinear Elliptic Boundary Value Problems. Japan Journal for Industrial and Applied Mathematics, Vol. 26, No. 2-3 (2009).
- [3] Nakao M.T., and Yamamoto, N.



Self-validating methods
Computer's challenge to the infinity
(Nihonhyoron-sha. 1998)