Dual Padé iterations and sentimental memories

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Outline

1. Part I - memories
   - Important people in my life
   - Conferences
   - Visitors in Wrocław
   - Castle
2. Part II - talk
   - Idea born in Leuven
   - p-sector function and pth root
   - Dual Padé iterations
   - Residuals and convergence
   - Series expansion of iterates
   - References
   - Appendix - after the talk

Important people in my life

Wrocław – town hall

My first boyfriend (on the left), KZ (on the right)
Warsaw 1943/1944

- He is 2 months older.
- Chemist, Polish Academy of Sciences, Warsaw
- Vice-President of Polish Academy of Sciences, 2003-2006
- Honorary Professor of Siberian Branch of Russian Academy of Sciences

Witold Roter (first row, first from the right)
KZ (second row, third from the left) Nowa Ruda 1957

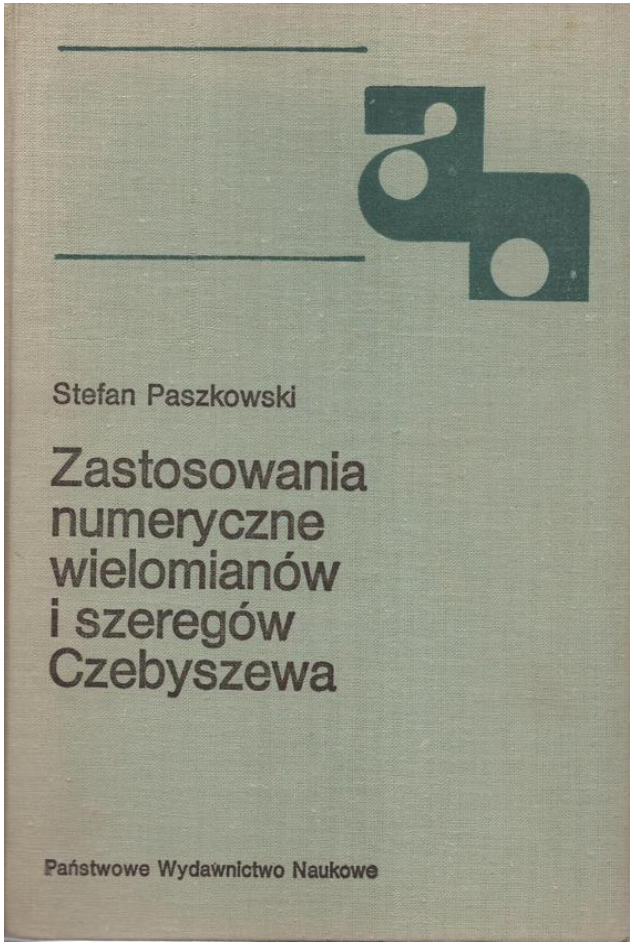
- My first teacher of mathematics in primary school
- Later, professor at University of Wrocław

Stefan Paszkowski, Wrocław 1992

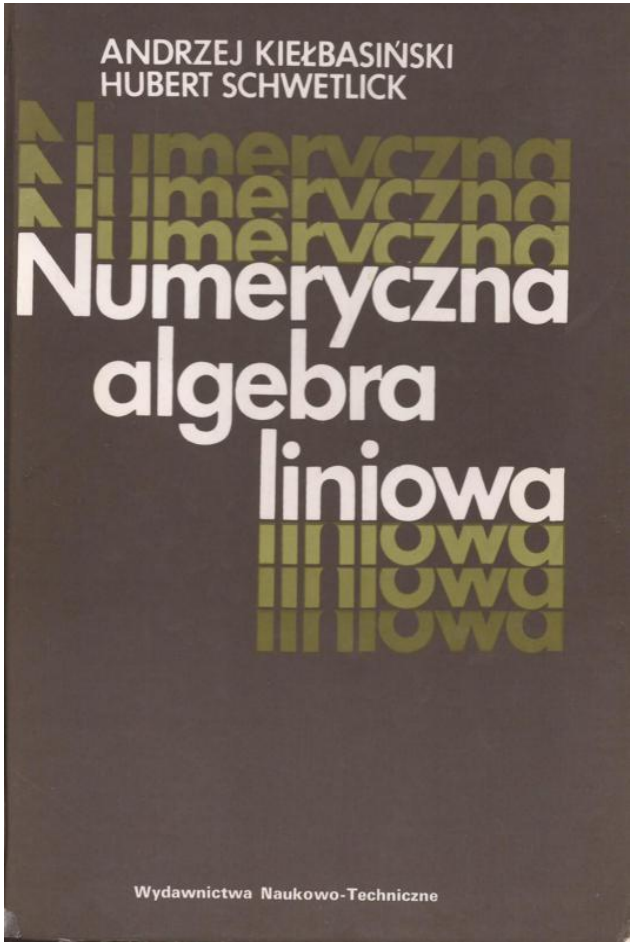
- Supervisor of my PhD dissertation
- 1962 – he established Cathedra of Numerical Methods, where an **English computer Elliott 803** was installed
- software: for *Polish computers produced by Elwro*
- *book*: Zastosowania numeryczne wielomianów i szeregów Czebyszewa

Stefan Paszkowski (on the left)
Andrzej Kiełbasiński (on the right)

- Kiełbasiński (professor at University of Warsaw) has translated into Polish Wilkinson's book
- *book*: A. Kiełbasiński, H. Schwetlick, Numeryczna Algebra Liniowa (German and Polish editions)

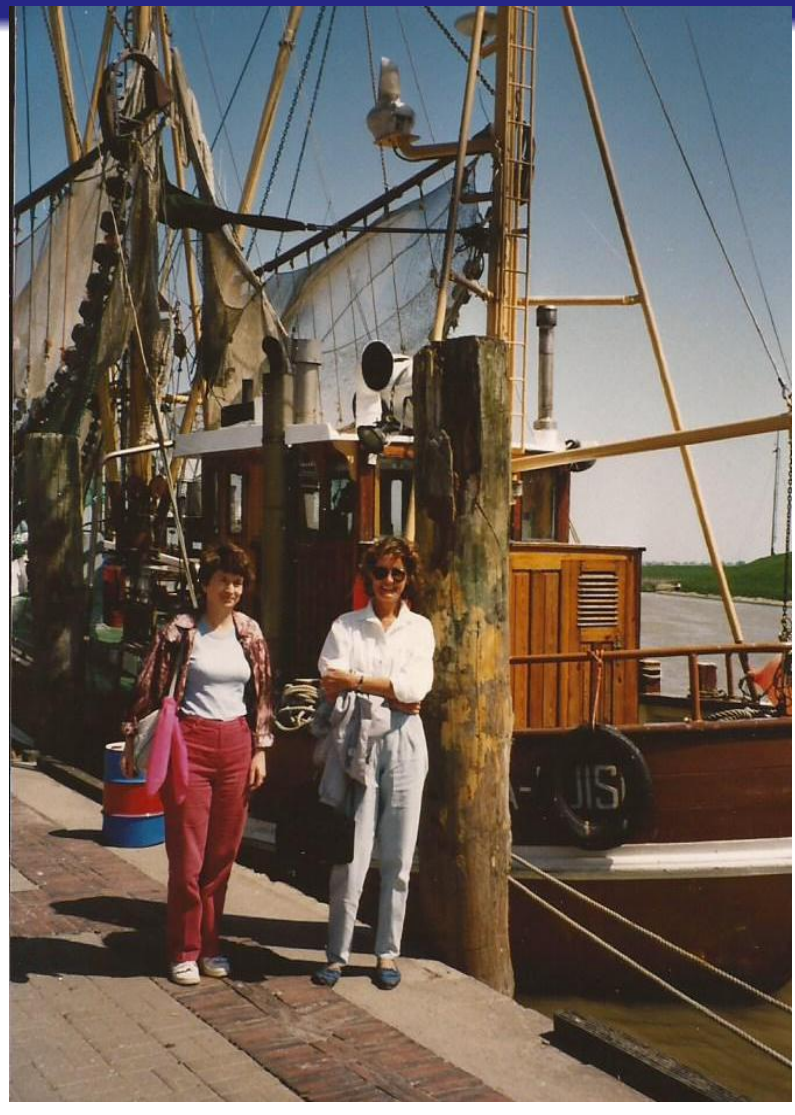


Warsaw 1975



German edition 1988
Polish editions 1992, 1994

Helmut Späth, Oldenburg (1986)



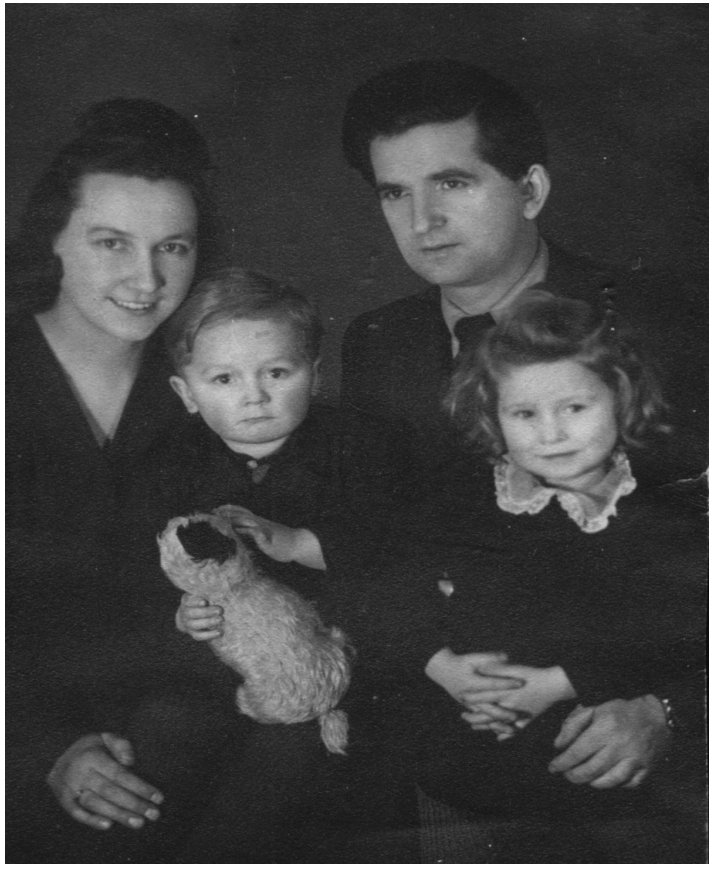
wife of Späth and sea (1988)

My first visit at a "western university" (4 days)
The second visit (1988) was 2 days longer.

Jacek Cichoń

- Professor at Wrocław University of Technology
- He applies advanced mathematics in computer science.
- The most popular teacher of informatics in our department.
- Financial support of my participation at conferences depends on him.

At last my parents, sister and brother



KZ on the right

KZ on the right

Conferences

Wrocław – opera

- Karl-Marx-Stadt (1982) – my first foreign conference
- Oberwolfach (1988)
  my first conference in "western country"
  invitation by Manfred von Golitschek

G. Meinardus, W. Hayman, F. Deutsch, L. Collatz
Oberwolfach 1988

Oberwolfach 1988

William Light and platform

Ward Cheney – Manfred von Golitschek – William Light

approximation in tensor product spaces

$AX + YB = C$, Chebyshev norm

UNIVERSITÄT HAMBURG

INSTITUT FÜR
ANGEWANDTE MATHEMATIK

Prof. Dr. L. Collatz

Institut für Angewandte Mathematik
2 Hamburg 13, Bundesstraße 55

Frau
Dr. K. Zietak
Institute of Computer Science
University of Wroclaw
ul. Przesmyckiego 20
PL-51-151 Wroclaw
Polen

Fernsprecher: 4123-4077 } Durchwahl
Behördennetz: 9.38.(„)
Telex-Nr.: 2 14732

Datum und Zeichen Ihres Schreibens | Aktenzeichen (bei Antwort bitte angeben.) Co/sch | Datum 13. Mai 1988

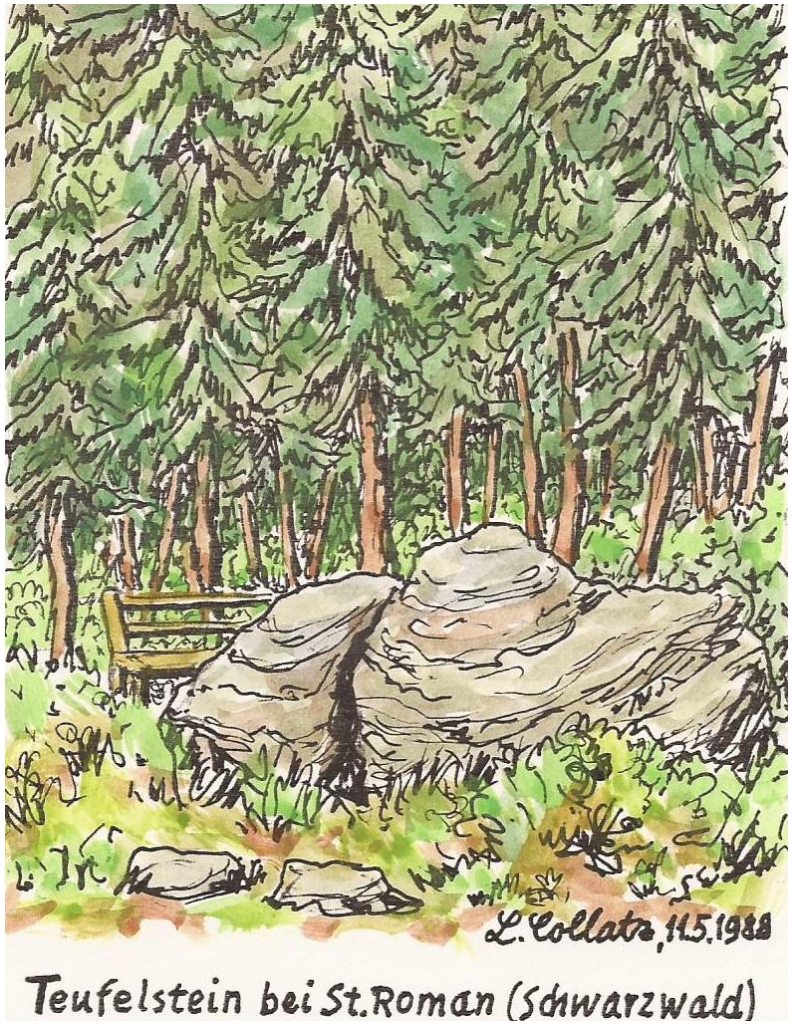
Betreff
Liebe Frau Zietak,

es hat mich sehr gefreut, in Oberwolfach Ihre Bekanntschaft gemacht und Gelegenheit gehabt zu haben, Sie auch persönlich etwas näher kennenzulernen; Sie haben ja auch die Wanderung so schön mitgemacht und so lege ich eine kleine Skizze bei, deren Beginn als Bleistiftzeichnung Sie in St. Roman sahen. Ihren Brief und Ihr Manuskript habe ich an Herrn Prof. Kielbasinski weitergegeben. Ich wünsche Ihnen für Ihre weitere wissenschaftliche Arbeit recht viel Erfolg, und daß Ihre geplante Reise nach England verwirklicht wird.

In der Hoffnung auf gelegentliches Wiedersehen bin ich mit herzlichen Grüßen
Ihr L. Collatz

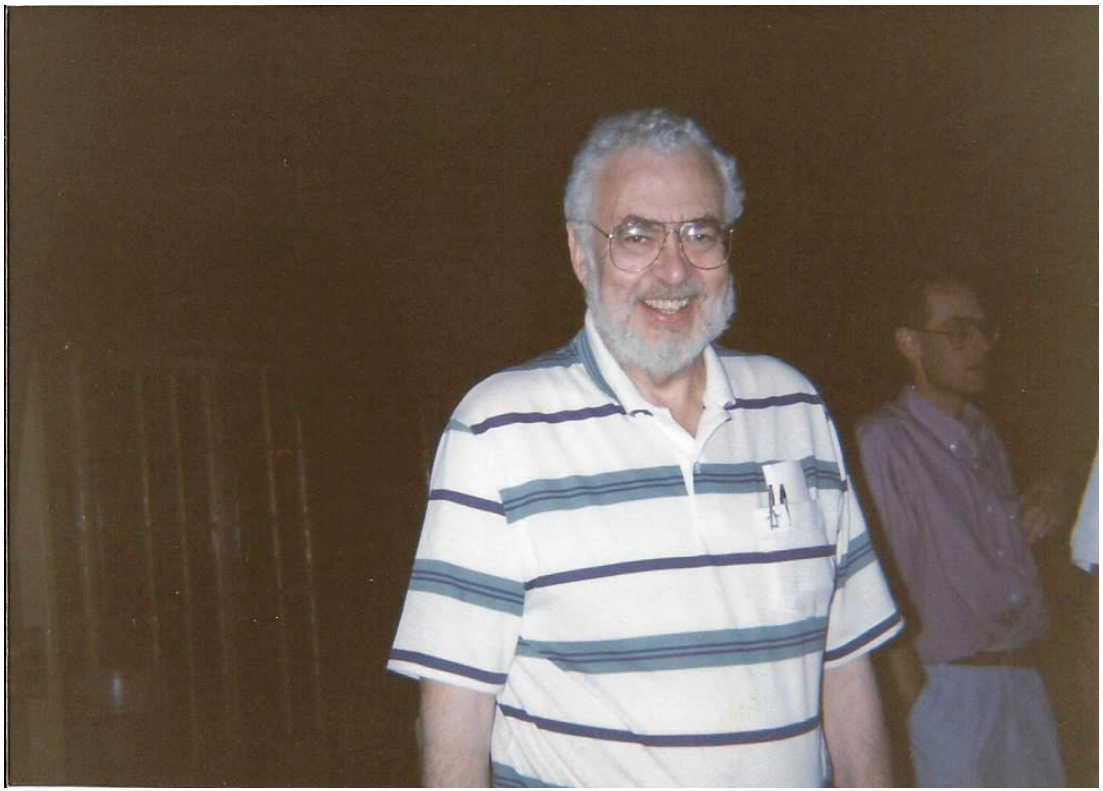
Herr Kielbasinski läßt Sie herzlich grüßen.

Entschuldigen Sie bitte, daß ich diesen Brief in Deutsch schreibe, ich hoffe, daß Sie jemanden haben, der den Brief übersetzen kann.



Letter and picture: Lothar Collatz, Oberwolfach 1988

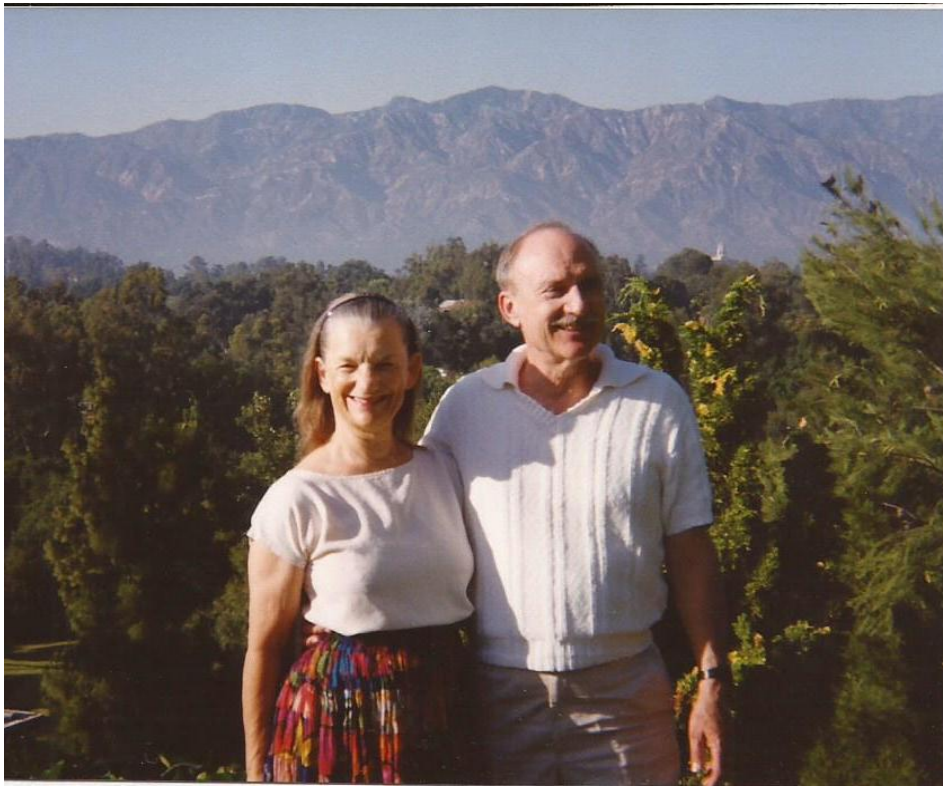
- 1989 – William Light (Lancaster)
  Alistair Watson (Dundee Conference)
- 1991 – Manchester (Nick Higham and Kung Kiu Lau)



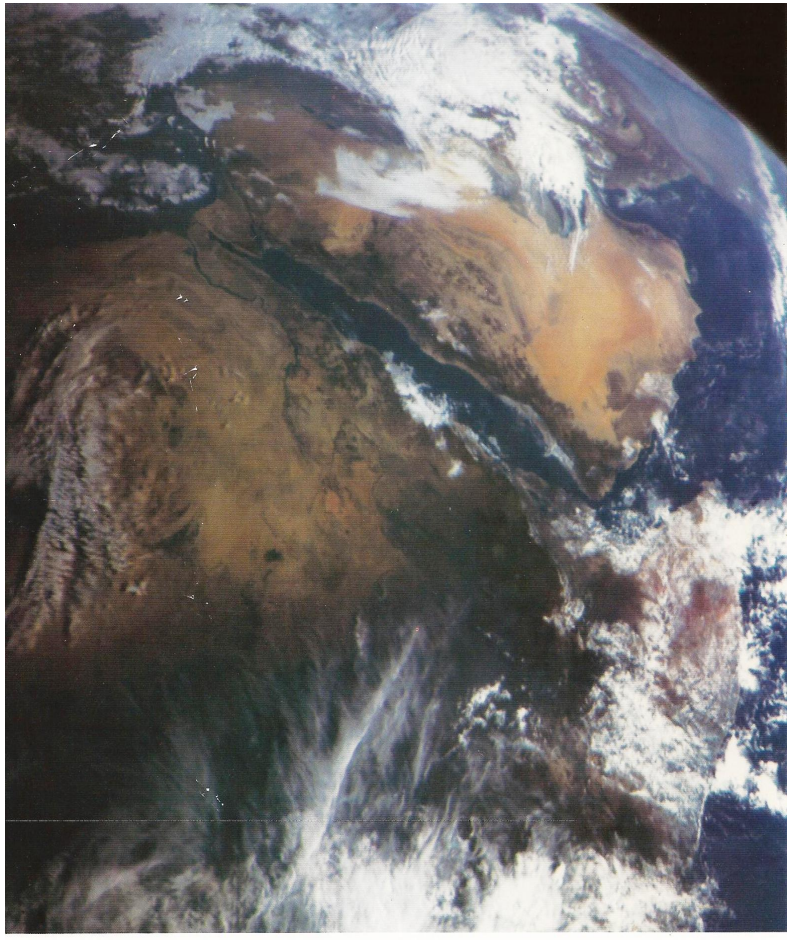
Householder Symposium, Lake Arrowhead (1993)
invitation by Gene Golub

Householder Symposium 1993

W. Proskurowski
Los Angeles, Beverly Hills



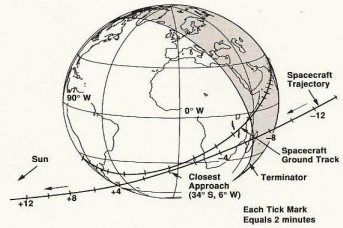
D. and Ch. Lawson
father day in Pasadena



G A L I L E O

The Near East
(P-41474)

This image of northeast Africa and the Arabian Peninsula was taken from an altitude of about 500,000 kilometers (300,000 miles) by the Galileo spacecraft on December 9, 1992, as it left Earth en route to Jupiter. Visible are most of Egypt (left of center), including the Nile Valley; the Red Sea (slightly above center); Israel; Jordan, and the Arabian Peninsula. In the center, below the coastal cloud, is Khartoum, at the confluence of the Blue Nile and the White Nile. Somalia (lower right) is partly covered by clouds.



During its second Earth encounter, the Galileo spacecraft passed within 305 kilometers (190 miles) of Earth's surface.

The Galileo Mission

The Galileo mission to Jupiter, sponsored by the National Aeronautics and Space Administration (NASA), will study the planet's atmosphere, satellites and surrounding magnetosphere. The spacecraft, consisting of an orbiter and an atmospheric entry probe, was launched aboard Space Shuttle Atlantis on October 18, 1989. The Jet Propulsion Laboratory of the California Institute of Technology designed and built the orbiter and is responsible for overall project management and mission operations. The probe was designed and built by Hughes Aircraft Company under contract to NASA's Ames Research Center. The propulsion module was provided by the Federal Republic of Germany. About 120 scientists from six nations are involved in the scientific mission.

To reach Jupiter, Galileo has flown a complex path. The spacecraft passed Venus on February 10, 1990, Earth on December 8, 1990, and Earth again on December 8, 1992, each encounter increasing its velocity relative to the Sun. This Venus–Earth–Earth gravity-assist (VEEGA) trajectory will extend more than 6 years from launch to arrival at Jupiter in December 1995. Along the way, the spacecraft has flown past Gaspra and will encounter Ida, two asteroids orbiting in the main asteroid belt between Mars and Jupiter — the first such flybys in solar system exploration.

When Galileo reaches Jupiter, the probe will descend through the Jovian clouds, transmitting its scientific measurements to Earth via the orbiter. Then the orbiter will begin a 2-year tour of Jupiter to study and map the major satellites — from as close as a few hundred kilometers — and to monitor the planet's atmosphere and magnetosphere.

NASA
National Aeronautics and Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

JPL 400-499E 4/93

Northeast Africa and Arabian Peninsula from 500 000 km
by **Galileo** spacecraft (NASA)
Ch. Lawson – Jet Propulsion Laboratory in Pasadena 1993

Lake Arrowhead (1993)

Tony Chan, Nick Higham, Valerie Fraysse, Haesun Park

polar decomposition, approximation of matrices
spectral portraits – MATLAB

Charles Van Loan, Sabine Van Huffel
Lake Arrowhead 1993

Valeria Simoncini
Whistler 1999

shared rooms
during Householder Symposiums in Peebles and Whistler

Whistler (1999)
V. Simoncini and B. Parlett

car in 1993: Gragg, Parlett

Pontresina (1996)
Nick Higham and Francoise Tisseur

in Alps

Whistler (1999)

Walter Gander with wife Heidi
Swiss chocolates

Chandler Davis with wife
conjectures
son Aaron, concert of Holly Cole in Wrocław

M. Overton and his mother
"Overton" hotel in Vancouver

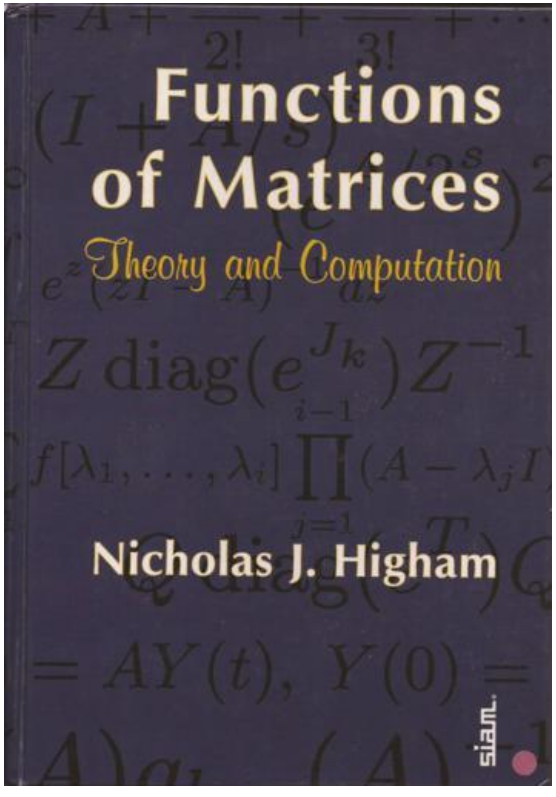
Vancouver 1999

N. Trefethen, Michele (wife of Overton)
M. Overton, Z. Strakos

Berlin-Zeuthen 2008

Nick Trefethen
Zeuthen - Berlin, 2008
Chebyshev polynomials

Peebles 2002
photo done by Nick Higham



Francoise Tisseur and Nick Higham
Householder Symposium, Berlin-Zeuthen 2008

gift: new book, SIAM 2008
the workshop *New Directions in Functions of Matrices*
Manchester 2008

J. Liesen, Berlin-Zeuthen 2008

P. Tichy, Valencia 2012

Application of approximation of matrices to GMRES

Van Dooren, Bhatia
ILAS, Chemnitz 1996

matrix analysis
positive definite matrices

Poloni, Meini, Iannazzo
Valencia 2012

some inspirations

Valencia 2012

Jennifer Scott

walks and talks

Dopico, Ipsen, Holodnak, Międlar
Mackey, Mackey
structure preserving

Leuven 2012

Dario Bini, Daniel Kressner

Froilán Dopico, Francoise Tisseur

structured matrices

GAMM in Gdańsk 2009 (minisymposium, Kressner and KZ)

Boston 2001

strict spectral approximation of matrices – conjecture

Gilbert Strang (see his home page)

I wish all of you to have such cupcakes!!!

Visitors in Wrocław

University of Wrocław – assembly hall

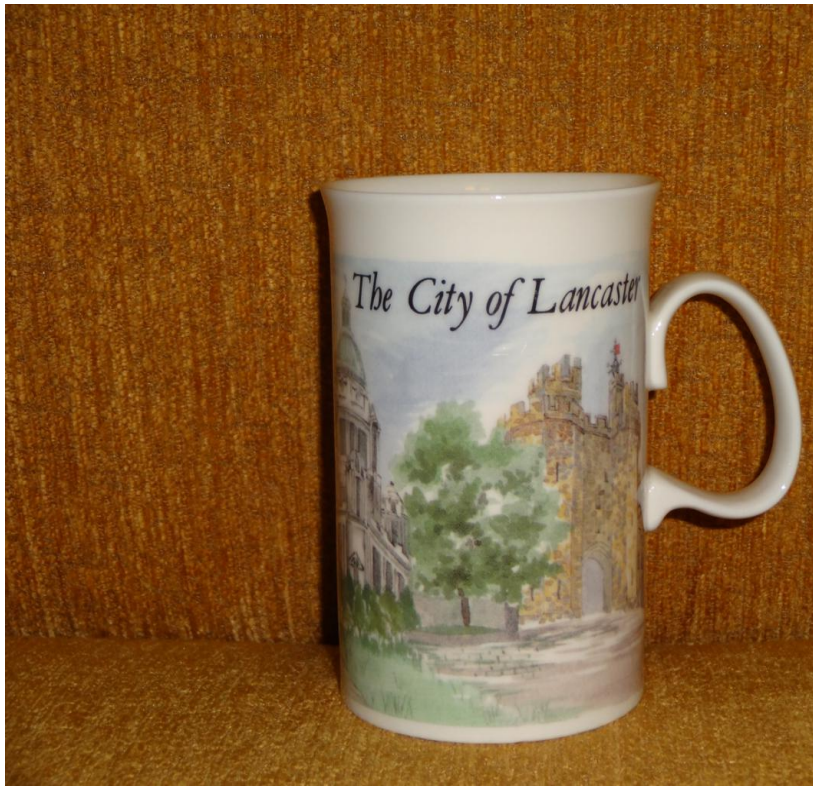
H. Späth
Wrocław - Książ (1987)

K.-K. Lau
Wrocław (1992)

Helena Krupicka, Alistair Watson
Wrocław (1988)

Alistair and his family

book: *Approximation Theory and Numerical Methods*



William Allan Light (Wrocław 1989)

(1950–2002)

gift: book of Cheney and Kincaid

Dottie and Chuck Lawson, and Poland in 1994

Ludwig Elsner, Jaroslav Zémanek (2000)

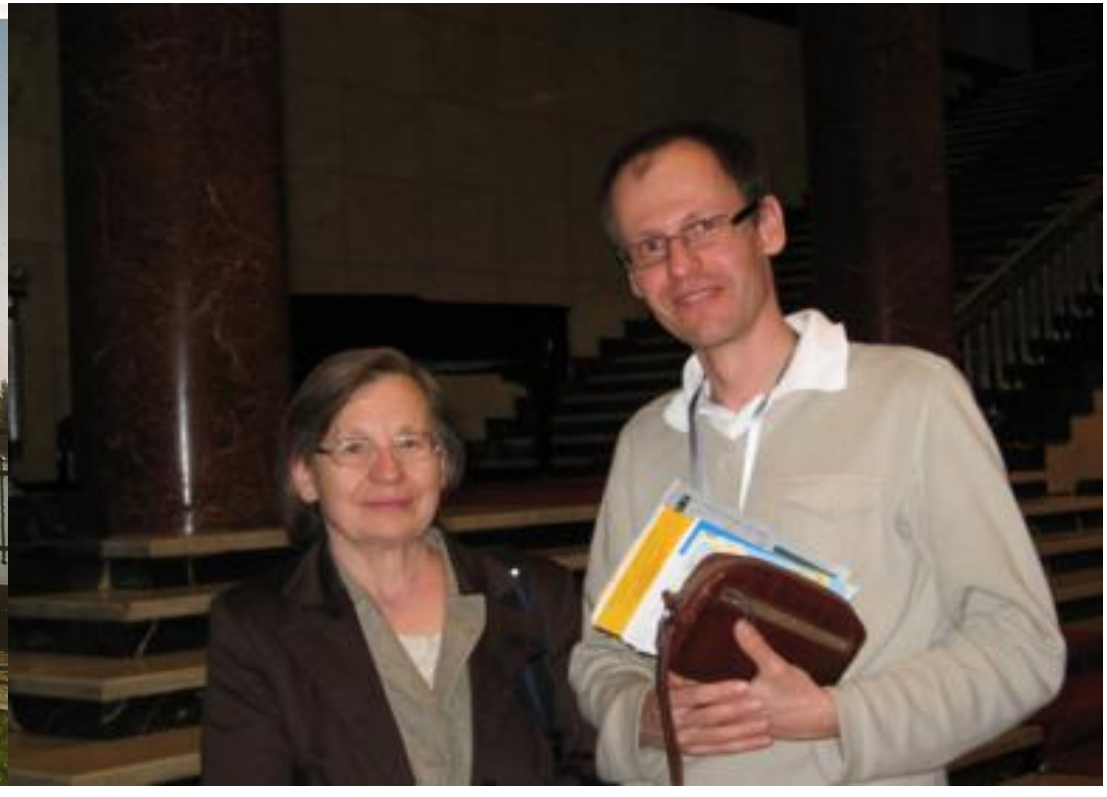
Wrocław
roots in ...

Jesse Barlow (2000, 2002)

museum of honey near Krynica

Charles Johnson
Wrocław

Matrix analysis



Ala Smoktunowicz, Miro Rozloznik
Novi Sad (2008)

Gram-Schmidt orthogonalization

German–Polish Workshop for Young Researches

Będlewo 2006

GAMM – Heike Fassbender, Volker Mehrmann, KZ

Volker Mehrmann
Whistler 1999

I.Wróbel, B.Laszkiewicz, A.Międlar
Będlewo 2006

Welcome to Książ Castle on rock cliff
Pearl of Lower Silesia

picture done by P. Kobylański

I would like to thank all of you
I have met on my "scientific" way!!!

Dual Padé iterations

My questions

- Why some properties of Newton's and Halley's methods, shown by Guo (2010) for computing matrix pth root, are common?
- Why Guo applies similar residuals to Newton's and Halley's methods for investigation of convergence?

My answer

- "Newton" is not Padé iteration, but "Halley" is.
- However, Newton's and Halley's methods are (new) dual Padé iterations.

Question of Iannazzo

How to generalize the reciprocal Padé iterations of Greco-Poloni-Iannazzo (for sign) to p-sector function?

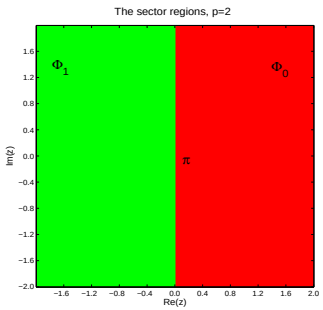
Padé iterations

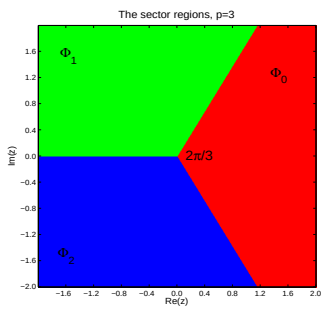
- sign function
  Kenney, Laub (1991)
- square root
  Higham (1997)
- square root
  Higham, Mackey, Mackey, Tisseur (2004)
- *p*-sector function and *p*th root
  Laszkiewicz, Zietak (2009)
- sign function
  reciprocal Padé iterations
  Greco-Poloni-Iannazzo (2012)
- *p*-sector function and *p*th root
  dual Padé iterations
  Zietak (2012)

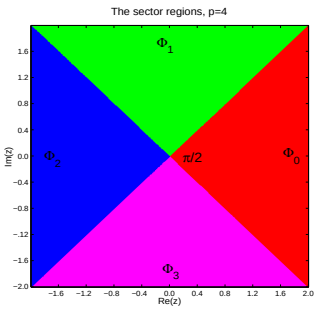
scalar *p*-sector function

$$\mathrm{sect}_p(z) = \frac{z}{\sqrt[p]{z^p}} \quad \text{the nearest } \textit{pth} \text{ root of unity to } z$$

$p = 2$ sign function







sectors

$$\Phi_k = \left\{ z \in \mathbb{C} : \frac{2k\pi}{p} - \frac{\pi}{p} < \arg(z) < \frac{2k\pi}{p} + \frac{\pi}{p} \right\}$$

Principal pth root and p-sector function

matrix principal pth root $A^{1/p}$ of A

no eigenvalue of A lies on closed negative real axis

$$X^p = A, \qquad \lambda_j(X) \in \Phi_0$$

matrix p-sector function of nonsingular A

$$\arg(\lambda_j(A)) \neq (2q+1)\pi/p, \qquad q = 0, 1, \ldots, p-1$$

$$\operatorname{sect}_p(A) = A(A^p)^{-1/p}$$

Padé approximants

$$\frac{P_{km}(z)}{Q_{km}(z)} = \frac{{}_2F_1\left(-k, \frac{1}{p} - m; -k - m; z\right)}{{}_2F_1\left(-m, -\frac{1}{p} - k; -k - m; z\right)}$$

$[k/m]$ Padé approximant to $f(z) = \frac{1}{(1-z)^{1/p}}$

$\frac{Q_{km}(z)}{P_{km}(z)}$ [m/k] Padé approximant

to $\frac{1}{f(z)} = (1-z)^{1/p}$

Matrix principal pth root

Padé

$$X_{j+1} = X_j \frac{P_{km}(I - A^{-1}X_j^p)}{Q_{km}(I - A^{-1}X_j^p)}, \qquad X_0 = I$$

Halley $k = m = 1$

dual Padé

$$Y_{j+1} = Y_j \frac{Q_{km}(I - AY_j^{-p})}{P_{km}(I - AY_j^{-p})}, \qquad Y_0 = I$$

Newton $k = 0, m = 1$, Halley $k = m = 1$
Schröder $k = 0, m$ arbitrary

coupled iterations

Matrix p-sector function

Padé

$$X_{j+1} = X_j \frac{P_{km}(I - X_j^p)}{Q_{km}(I - X_j^p)}, \qquad X_0 = A$$

dual Padé

$$Y_{j+1} = Y_j \frac{Q_{km}(I - Y_j^{-p})}{P_{km}(I - Y_j^{-p})}, \qquad Y_0 = A$$

matrix pure iterations

reciprocal Padé for sign (Poloni-Greco-Iannazzo)

$$Y_{j+1} = \frac{Q_{km}(I - Y_j^2)}{Y_j P_{km}(I - Y_j^2)}, \qquad Y_0 = A$$

dual Padé for sign $(p = 2)$

$$Y_{j+1} = \frac{Y_j Q_{km}(I - Y_j^{-2})}{P_{km}(I - Y_j^{-2})}, \qquad Y_0 = A$$

Residuals for pth root

Padé $X_{j+1} = X_j \frac{P_{km}(I - A^{-1}X_j^p)}{Q_{km}(I - A^{-1}X_j^p)}, \qquad X_0 = I$

$$S_\ell = I - A^{-1}X_\ell^p$$

$$S_{\ell+1} = f_{km}(S_\ell)$$

dual Padé $Y_{j+1} = Y_j \frac{Q_{km}(I - AY_j^{-p})}{P_{km}(I - AY_j^{-p})}, \qquad Y_0 = I$

$$R_\ell = I - AY_\ell^{-p}$$

$$R_{\ell+1} = f_{km}(R_\ell)$$

Guo (2010) – R_ℓ for Newton and Halley

Principal Padé iterations

for $[k/k]$

principal Padé and principal dual Padé iterations

$$S_\ell = I - A^{-1} X_\ell^p$$

$$S_{\ell+1} = f_{kk}(S_\ell)$$

$$R_\ell = I - A X_\ell^{-p}$$

$$R_{\ell+1} = f_{kk}(R_\ell)$$

answer to the question

Certain regions of convergence

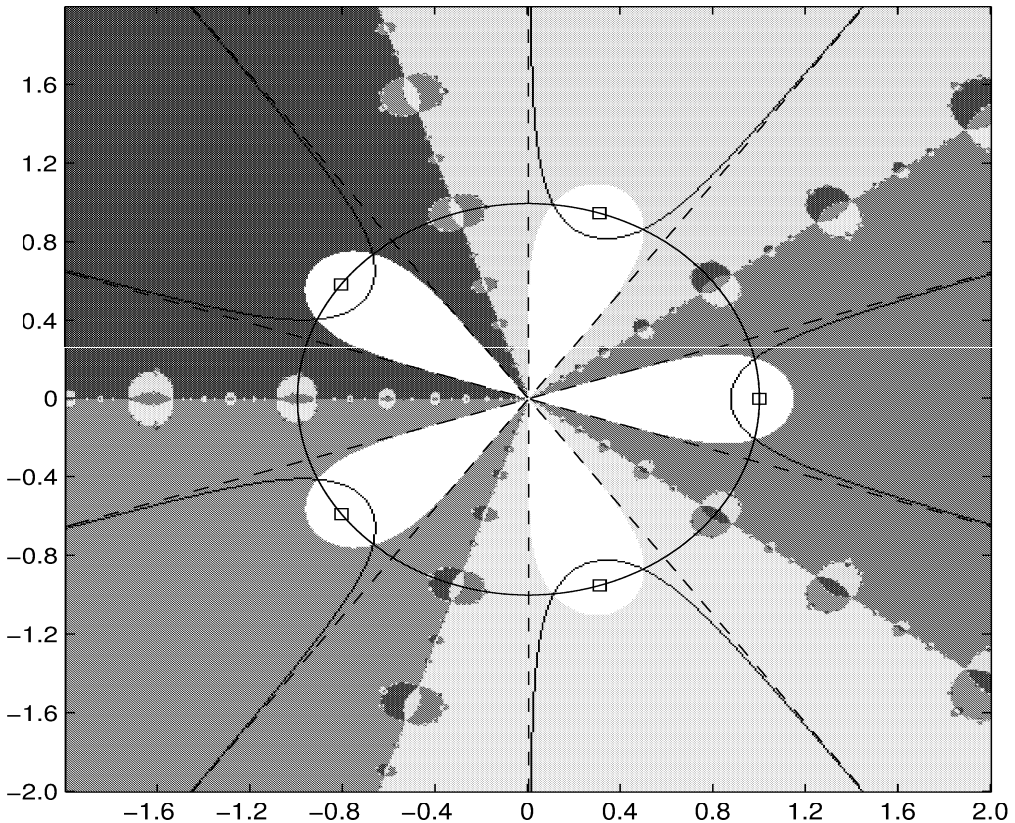
$\lambda_j(A)$ in regions:

$$\mathbb{L}_p = \{z \in \mathbb{C} : |1 - z^p| < 1\} \quad \textit{Padé for } p - \textit{sector}, X_0 = A$$

$$\mathbb{L}_{-p} = \{z \in \mathbb{C} : |1 - z^{-p}| < 1\} \quad \textit{dual Padé for } p - \textit{sector}, X_0 = A$$

$$\mathbb{K} = \left\{ z \in \mathbb{C} : \left| 1 - \frac{1}{z} \right| < 1 \right\} \quad \textit{Padé for } p\text{th root}, X_0 = I$$

$$\mathbb{M} = \{z \in \mathbb{C} : |1 - z| < 1 \} \quad \textit{dual Padé for } p\text{th root}, X_0 = I$$



$p = 5$, Halley iterations for p-sector function,

$\mathbb{L}_{-p}^{(Padé)}$ (solid contour), $\mathbb{L}_{p}^{(Padé)}$ (white flower)

$\mathbb{B}_{p}^{(Hall)}$ (dash contour)

Crucial function – arbitrary integers k, m

$$f_{km}(z) = 1 - (1-z)\left(\frac{P_{km}(z)}{Q_{km}(z)}\right)^p$$

all Taylor coefficients of $f_{km}(z)$ are positive !!!

$f_{km}(1) = 1$

Oleksandr Gomilko, Minghua Lin, Dmitry Karp, KZ (2012)

Gomilko, Greco, KZ (2012)

$$\frac{P_{km}(z)}{Q_{km}(z)} \qquad [k/m] \text{ Padé approximant}$$

$$\text{to} \quad \frac{1}{(1-z)^{1/p}}$$

Positivity of coefficients of $f_{km}(z)$

Particular cases:

Guo (2010)

Newton's method $f_{01}(z)$ $k = 0, m = 1$

Minghua Lin (2010)

Halley's method $f_{11}(z)$ $k = m = 1$

Cardoso and Loureiro (2011)

Schröder's iterations
$f_{0m}(z)$ $k = 0,$ m arbitrary

Binomial expansion

$$(1-z)^{1/p} = \sum_{j=0}^{\infty} \beta_j z^j$$

dual $[k/m]$ Padé iterate Y_ℓ for computing matrix pth root $(I-B)^{1/p}$

$$Y_\ell = \sum_{j=0}^{\infty} \varphi_{km,j}^{(\ell)} B^j$$

$$\varphi_{km,j}^{(\ell)} = \beta_j \qquad j = 0, \ldots, (k+m+1)^\ell - 1$$

Guo (2010) – Newton and Halley

Summary

- New families of dual Padé iterations for computing matrix pth root and matrix p-sector function have been introduced.
- Certain regions of convergence have been determined.
- A certain property proved by Guo for iterates generated by Newton's and Halley's methods for computing $(I - B)^{1/p}$ holds also for iterates generated by the dual Padé methods.

References I

- **Cardoso, Loureiro**, On the convergence of Schröder iteration function for the *p*th roots of complex numbers, *Applied Math. Comput.* (2011).
- **Greco, Iannazzo, Poloni**, The Padé iterations for the matrix sign function and their reciprocal are optimal, *Lin. Alg. Appl.* (2012).
- **Guo**, On Newton's and Halley's method for the principal *p*th root of a matrix, *Lin. Alg. Appl.* (2010).
- **Higham**, Stable iterations for the matrix square root, *Numer. Alg.* (1997).

References II

- **Higham, Mackey, Mackey, Tisseur**, Computing the polar decomposition and the matrix sign decomposition in matrix group, *SIAM J. Matrix Anal.* 25 (2004).
- **Kenney, Laub**, Rational iterative methods for the matrix sign function, *SIAM J. Matrix Anal. Appl.* 12 (1991).
- **Minghua Lin**, A residual recurrence for Halley's method for the matrix pth root, *Lin. Alg. Appl.* (2010).

References III

- **Gomilko, Greco, Ziętak,** A Padé family of iterations for the matrix sign function and related problems, *Numer. Lin. Alg. Appl.* (2011).
- **Gomilko, Karp, Lin, Ziętak,** Regions of convergence of a Padé family of iterations for the matrix sector function, *J. Comput. Appl. Math.* (2012).
- **Laszkiewicz, Ziętak,** A Padé family of iterations for the matrix sector function and the matrix pth root, *Numer. Lin. Alg. Appl.* (2009).
- **Ziętak**, The dual Padé families of iterations for the matrix pth root and the matrix p-sector function, *J. Comput. Appl. Math.*, submitted.

Appendix

After the talk

Bhatia, Bini, Guo, Higham, Iannazzo, Ipsen, Meini, Poloni, Simoncini, Tisseur, Trefethen, Van Loan, and KZ

Manchester, April 11, 2013

Thank you!

Wrocław the city of DWARFS