The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2042-5

Co-sponsored School/Workshop on Integrable Systems and Scientific Computing

15 - 20 June 2009

Convergence Analysis of Exponential Integrators

Alexander Ostermann
Universität Innsbruck
Austria

e-Mail: alexander.ostermann@uibk.ac.at

Convergence Analysis of Exponential Integrators

Alexander Ostermann
Universität Innsbruck, Austria

School/Workshop on
Integrable Systems and Scientific Computing

Trieste, 18/19 June 2009

joint work with Marlis Hochbruck, Düsseldorf

Outline

Introduction

Linear problems

Semilinear problems

Exponential Rosenbrock-type methods

Implementation of exponential integrators

Exponential meshless methods

Motto: evolutionary PDE = abstract ODE

In 1971, I read the beautiful paper of Kato and Fujita on the Navier-Stokes equation [sic!] *and was delighted to find that, properly viewed, it looked like an ordinary differential equation, and the analysis proceeded in ways familiar to ODEs.*

Dan Henry,
Geometric theory of semilinear parabolic equations (1981)

Abstract formulation: example

$$\frac{\partial U}{\partial t}(x,t) = \frac{\partial}{\partial x}\left(a(x)\,\frac{\partial U}{\partial x}(x,t)\right) + \Phi\big(x,t\big)$$

$$U(x,0) = U_0(x) \qquad\qquad 0 < x < 1$$

$$U(0,t) = U(1,t) = 0 \qquad\qquad t > 0$$

consider:

$$u(t) = [x \mapsto U(x,t)], \qquad g(t) = \big[x \mapsto \Phi\big(x,t\big)\big]$$

$$Av = \left[x \mapsto \frac{\partial}{\partial x}\left(a(x)\,\frac{\partial v}{\partial x}\right)\right] \qquad \text{unbounded operator}$$

gives: $\qquad u' = Au + g(t), \qquad u(0) = u_0 \qquad \text{on} \quad X$

Outline

Linear parabolic problem

Linear problem

$$u' = Au + g(t), \quad u(0) = u_0$$

variation-of-constants formula

$$u(t) = \mathrm{e}^{tA} u_0 + \int_0^t \mathrm{e}^{(t-\tau)A} g(\tau)\,\mathrm{d}\tau$$

Taylor series expansion

$$g(\tau) = g(0) + \int_0^\tau g'(s)\,\mathrm{d}s$$

yields

$$u(h) = \mathrm{e}^{hA} u_0 + \int_0^h \mathrm{e}^{(h-\tau)A} g(0)\,\mathrm{d}\tau + \mathcal{O}(h^2)$$

φ-function and Exponential Euler method

Exact solution at $t_{n+1} = t_n + h$

$$u(t_{n+1}) = \mathrm{e}^{hA}u(t_n) + \int_0^h \mathrm{e}^{(h-s)A}g(t_n)\mathrm{d}s + h^2\delta_{n+1}$$

$$= \mathrm{e}^{hA}u(t_n) + h\varphi_1(hA)g(t_n) + h^2\delta_{n+1}$$

with φ-function

$$\varphi_1(tA) = \frac{1}{t}\int_0^t \mathrm{e}^{(t-s)A}\mathrm{d}s$$

Exponential Euler method

$$u_{n+1} = \mathrm{e}^{hA}u_n + h\varphi_1(hA)g(t_n)$$

Convergence

Theorem. The exponential Euler method has order one, i.e.,

$$\|u_{n+1} - u(t_{n+1})\| \le Ch$$

on compact time intervals $0 \le hn \le T$.

Proof. Error recursion

$$E_{n+1} = u_{n+1} - u(t_{n+1}) = \mathrm{e}^{hA} E_n - h^2 \delta_{n+1}$$

hence

$$E_n = \mathrm{e}^{nhA} E_0 - h^2 \sum_{j=0}^{n-1} \mathrm{e}^{(n-j-1)hA} \delta_{j+1}$$

Stability bound

$$\|\mathrm{e}^{tA}\| \le C\mathrm{e}^{\omega t}$$

Better approximations

Variation-of-constants formula

$$u(t) = \mathrm{e}^{tA} u_0 + \int_0^t \mathrm{e}^{(t-\tau)A} g(\tau)\mathrm{d}\tau$$

Taylor series expansion

$$g(\tau) = g(0) + \tau g'(0) + \int_0^\tau (\tau - s) g''(s)\mathrm{d}s$$

yields

$$u(h) = \mathrm{e}^{hA} u_0 + \int_0^h \mathrm{e}^{(h-s)A} g(0)\mathrm{d}s + \int_0^h \mathrm{e}^{(h-s)A} s\, g'(0)\mathrm{d}s + \mathcal{O}(h^3)$$

φ-functions and second order method

Let

$$\varphi_k(tA) = \frac{1}{t^k}\int_0^t \mathrm{e}^{(t-s)A}\frac{s^{k-1}}{(k-1)!}\,\mathrm{d}s, \qquad k \ge 1$$

with bounds

$$\|\varphi_k(tA)\| \le C\mathrm{e}^{\omega t}$$

Exact solution has the form

$$u(t_{n+1}) = \mathrm{e}^{tA}u(t_n) + h\varphi_1(hA)g(t_n) + h^2\varphi_2(hA)g'(t_n) + h^3\delta_{n+1}$$

Numerical approximation by interpolation

$$g(t_n+s) \approx g(t_n) + \frac{s}{h}\big(g(t_{n+1}) - g(t_n)\big), \qquad 0 \le s \le h$$

yields second order method

$$u_{n+1} = \mathrm{e}^{hA}u_n + h\big(\varphi_1(hA) - \varphi_2(hA)\big)g(t_n) + h\varphi_2(hA)g(t_{n+1})$$

Exponential quadrature rules

Linear problem

$$u' = Au + g(t), \quad u(0) = u_0$$

Numerical method

$$u_{n+1} = \mathrm{e}^{hA} u_n + h \sum_{i=1}^{s} b_i(hA)\, g(t_n + c_i h).$$

The underlying quadrature rule (i.e. for $A = 0$) has the weights $b_i(0)$. As usual, we require $c_i \neq c_j \quad \text{for} \quad i \neq j$.

Example: $s = 1,\ c_1 = 0,\ b_1(hA) = \varphi_1(hA)$

Example: $s = 2,\ c_1 = 0,\ c_2 = 1$

$$b_1(hA) = \varphi_1(hA) - \varphi_2(hA), \quad b_2(hA) = \varphi_2(hA)$$

Second order methods

Order conditions for order two

$$b_1(z) + \ldots + b_s(z) = \varphi_1(z)$$
$$b_1(z)c_1 + \ldots + b_s(z)c_s = \varphi_2(z)$$

Example: $s = 2,\ c_1 = 0,\ c_2 = 1$

$$b_1(z) = \varphi_1(z) - \varphi_2(z), \quad b_2(z) = \varphi_2(z)$$

How about superconvergence?

Example: Midpoint rule

$$s = 1, \qquad b_1(z) = \varphi_1(z), \quad c_1 = \frac{1}{2}$$

has classical order 2.

Superconvergence

Midpoint rule

$$u_{n+1} = \mathrm{e}^{hA} u_n + h\,\varphi_1(hA)\, g(t_n + \tfrac{h}{2})$$

Taylor expansion

$$h\varphi_1(hA)\, g(t_n + \tfrac{h}{2}) = h\varphi_1(hA)\, g(t_n) + \frac{h^2}{2}\varphi_1(hA)\, g'(t_n)$$

Note that

$$\begin{aligned} \varphi_2(z) &= \frac{1}{2} - z\varphi_3(z) \\ \frac{1}{2}\varphi_1(z) &= \frac{1}{2} - \frac{z}{2}\varphi_2(z) \end{aligned}$$

therefore

$$\varphi_2(hA) - \frac{1}{2}\varphi_1(hA) = -hA\Big(\varphi_3(hA) - \frac{1}{2}\varphi_2(hA)\Big)$$

Parabolic smoothing property

Smoothing property for $\alpha \geq 0$

$$\left\| (-A)^\alpha \mathrm{e}^{tA} \right\| \leq \frac{C}{t^\alpha} \mathrm{e}^{\omega t}, \quad t > 0$$

Additional term in error recursion

$$h^3 \sum_{j=0}^{n-1} \mathrm{e}^{(n-j-1)hA} A \Big(\varphi_3(hA) - \tfrac{1}{2} \varphi_2(hA) \Big) g'(t_j)$$

has the bound

$$C\, h^2 (1 + |\log h|) \qquad \text{or even} \qquad Ch^2$$

Exponential quadrature rules

Let the method

$$u_{n+1} = \mathrm{e}^{hA} u_n + h \sum_{i=1}^{s} b_i(hA)\, g(t_n + c_i h).$$

satisfy the order conditions

$$b_1(z)c_1^{q-1} + \ldots + b_s(z)c_s^{q-1} = \varphi_q(z), \qquad 1 \le q \le s$$

Theorem. If the underlying s-stage quadrature formula is of order $p \ge s$, then $\|u_n - u(t_n)\| \le C \cdot h^{\min(p,s+1+\beta)}$.

Condition on β: $\quad (-A)^{\beta} g^{(s+1)} \in L^1(0,T;X)$
typical value in L^2: $\quad \beta = 0.24999$
(for second order strongly elliptic operator)

Numerical example

Linear parabolic problem $(Av = \partial_{xx} v$, Dirichlet b.c.)

$$\frac{\partial U}{\partial t}(x,t) = \frac{\partial^2 U}{\partial x^2}(x,t) + \big(2 + x(1-x)\big)\mathrm{e}^t$$

with exact solution $U(x,t) = x(1-x)\,\mathrm{e}^t$. Standard finite differences for $0 \le x \le 1$.

Apply exponential 2-stage Gauss method with $h = 1/128$

d.o.f.	H^1	L^1	L^2	L^∞
50	2.80	3.53	3.27	3.00
100	2.76	3.50	3.26	3.01
200	2.75	3.50	3.25	3.00

Numerically observed orders of convergence at $t = 1$.

Stiffness takes its toll.

Outline

Exponential forward Euler method

Semilinear parabolic problem $u' = Au + f(u), \quad u(0) = u_0$

True solution (variation-of-constants formula)

$$u(t_{n+1}) = \mathrm{e}^{hA} u(t_n) + \int_0^h \mathrm{e}^{(h-\tau)A} f\big(u(t_n+\tau)\big)\,\mathrm{d}\tau$$

Approximate $f\big(u(t_n+\tau)\big) \approx f(u_n)$

$$u_{n+1} = \mathrm{e}^{hA} u_n + h\,\varphi_1(hA)\,f(u_n)$$

with

$$\varphi_1(hA) = \frac{1}{h}\int_0^h \mathrm{e}^{(h-\tau)A}\mathrm{d}\tau, \qquad \varphi_1(z) = \frac{\mathrm{e}^z - 1}{z}.$$

Convergence proof

Theorem. The exponential Euler method is first order convergent.

Proof. Insert the exact solution into the numerical scheme

$$\begin{aligned} u_{n+1} &= \mathrm{e}^{hA} u_n + h\varphi_1(hA)\, f(u_n) \\ u(t_{n+1}) &= \mathrm{e}^{hA} u(t_n) + h\varphi_1(hA)\, f(u(t_n)) - \delta_{n+1} \end{aligned}$$

with defects $\quad \|\delta_{n+1}\|_V \leq C \cdot h^2.$

This implies the error recursion $\; E_n = u_n - u(t_n)$

$$E_n = h \sum_{j=0}^{n-1} \mathrm{e}^{(n-j-1)hA} \varphi_1(hA)\, \Delta f_j + \sum_{j=0}^{n-1} \mathrm{e}^{(n-j-1)hA} \delta_{j+1}.$$

Convergence proof, cont.

We solve the error recursion

$$E_n = h \sum_{j=0}^{n-1} \mathrm{e}^{(n-j-1)hA} \varphi_1(hA)\, \Delta f_j + \sum_{j=0}^{n-1} \mathrm{e}^{(n-j-1)hA} \delta_{j+1}$$

and use the stability of the evolution and the Lipschitz condition on f

$$\|\mathrm{e}^{(n-j-1)hA} \varphi_1(hA)\, \Delta f_j\|_V \le C \cdot t_{n-j}^{-\alpha} \cdot \|E_j\|_V$$

Solving

$$\|E_n\|_V \le C\, h \sum_{j=0}^{n-1} t_{n-j}^{-\alpha} \|E_j\|_V + C\, h$$

by a discrete Gronwall lemma for weakly singular kernels concludes the proof.

Gronwall lemma – weakly singular kernels

Lemma. For $h > 0$ and $T > 0$, let $0 \le t_n = nh \le T$. Further assume that the sequence of non-negative numbers ε_n satisfies the inequality

$$\varepsilon_n \;\le\; ah \sum_{\nu=1}^{n-1} t_{n-\nu}^{-\rho} \varepsilon_\nu + b\, t_n^{-\sigma}$$

for $0 \le \rho < 1$ and $a, b \ge 0$. Then the following estimate holds

$$\varepsilon_n \;\le\; \begin{cases} Cb\, t_n^{-\sigma} & \text{for } \; 0 \le \sigma < 1, \\ Cb\big(t_n^{-1} + t_n^{-\rho}\, |\log h|\,\big) & \text{for } \; \sigma = 1, \end{cases}$$

where the constant C depends on ρ, σ, a, and on T.

Explicit exponential Runge–Kutta methods

An *explicit* exponential Runge–Kutta method, applied to $u' = Au + f(u)$, has the form

$$U_{ni} = \mathrm{e}^{c_i hA} u_n + h \sum_{j=1}^{i-1} a_{ij}(c_i hA)\, f(U_{nj}),$$

$$u_{n+1} = \mathrm{e}^{hA} u_n + h \sum_{i=1}^{s} b_i(hA)\, f(U_{ni}).$$

The coefficients b_i, a_{ij} are *linear* combinations of the functions $\varphi_1, \ldots, \varphi_s$, where

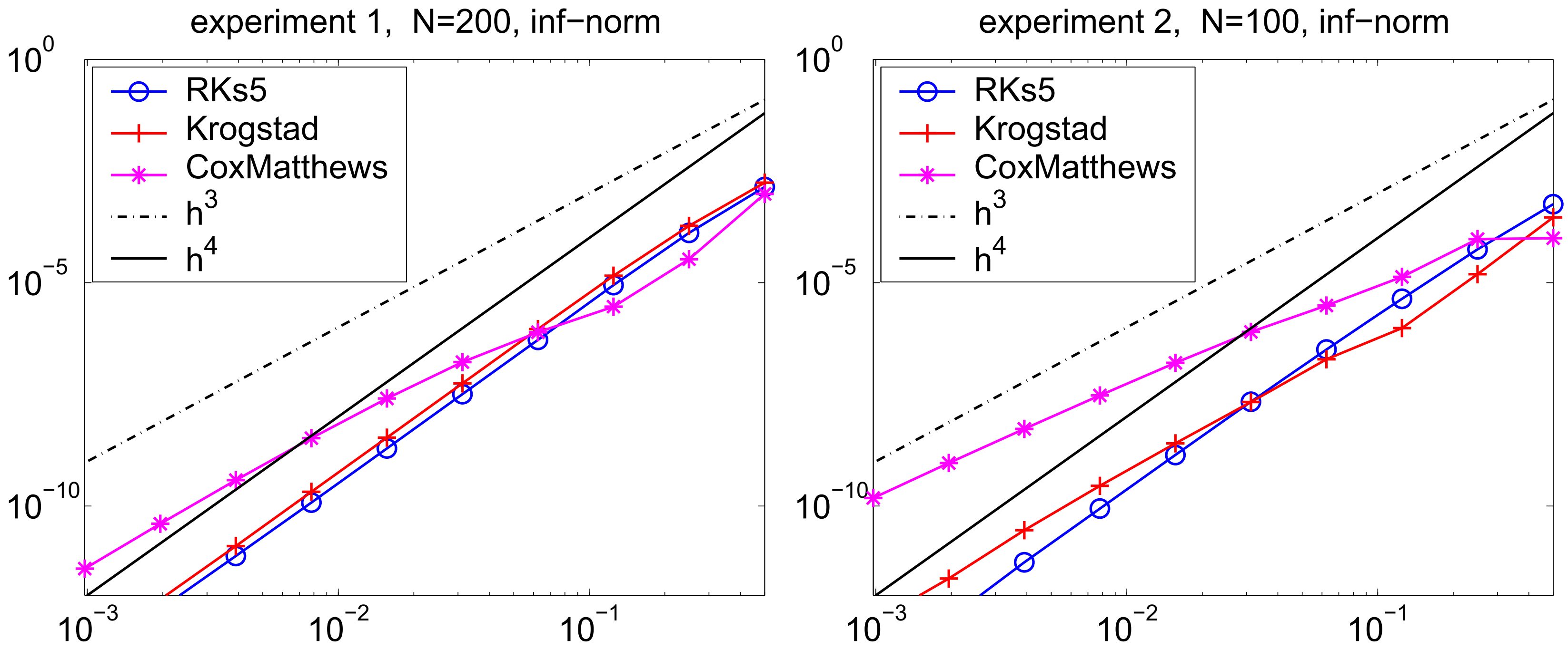
$$\varphi_k(hA) = h^{-k} \int_0^h \mathrm{e}^{(h-\tau)A} \frac{\tau^{k-1}}{(k-1)!}\, \mathrm{d}\tau$$

are *bounded* operators.

Stiff order conditions

No.	order	order condition
1	1	$\sum_{i=1}^{s} b_i(hA) = \varphi_1(hA)$ ✓
2	2	$\sum_{i=2}^{s} b_i(hA)c_i = \varphi_2(hA)$
3	2	$\sum_{j=1}^{i-1} a_{ij}(hA) = c_i\varphi_1(c_i hA), \quad i = 2, \dots, s$ ✓
4	3	$\sum_{i=2}^{s} b_i(hA)c_i^2 = 2\varphi_3(hA)$
5	3	$\sum_{i=2}^{s} b_i(hA)J\Big(\varphi_2(c_i hA)c_i^2 - \sum_{j=2}^{i-1} a_{ij}(hA)c_j\Big) = 0$
6	4	$\sum_{i=2}^{s} b_i(hA)c_i^3 = 6\varphi_4(hA)$
7	4	$\sum_{i=2}^{s} b_i(hA)J\Big(\varphi_3(c_i hA)c_i^3 - \frac{1}{2}\sum_{j=2}^{i-1} a_{ij}(hA)c_j^2\Big) = 0$
8	4	$\sum_{i=1}^{s} b_i(hA)J\sum_{j=2}^{i-1} a_{ij}(hA)J\psi_{2,j}(hA) = 0$
9	4	$\sum_{i=2}^{s} b_i(hA)c_i K\Big(\varphi_2(c_i hA)c_i^2 - \sum_{j=2}^{i-1} a_{ij}(hA)c_j\Big) = 0$

Numerical experiment



Maximum norm of errors for different methods of classical order four. In the first experiment, the operator $A^{-1}JA$ is bounded, whereas in the second one, only $A^{-1}JA^{1/2}$ is bounded.

Higher-order Runge–Kutta type methods

Explicit exponential RK methods up to order 4 have been constructed (Hochbruck, O., 2005)

- Stiff order conditions, convergence proofs.
- There exist methods of order 3 with 3 stages.
- For order 4, one needs at least 5 stages.

In a similar way, exponential multistep methods as well as exponential general linear methods have been derived (Calvo, Palencia, 2006; O., Thalhammer, Wright, 2006)

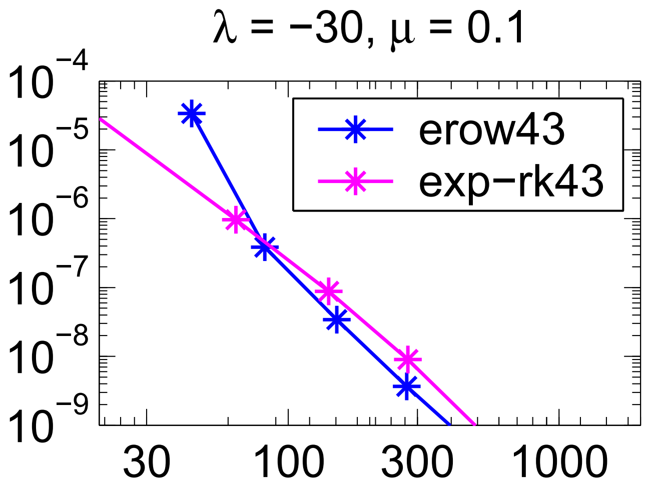
All methods make use of the φ-functions.

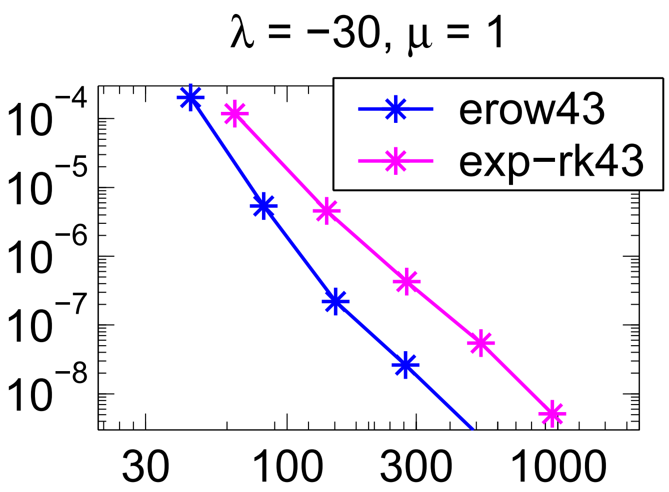
Methods are not invariant under linearisation

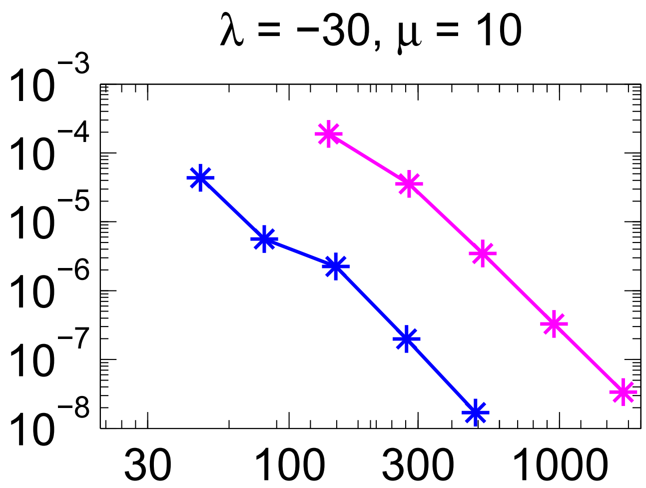
test problem

$$u' = \lambda u + \mu u^2 + k(t)$$
$$0 \le t \le 10$$

$$u(t) = \cos t$$







Outline

Introduction

Linear problems

Semilinear problems

Exponential Rosenbrock-type methods

Implementation of exponential integrators

Exponential meshless methods

Exponential integrators of Rosenbrock type

These integrators are based on the following ideas:

- Linearise the problem $u' = F(u), \quad u(0) = u_0$
  in each step at the initial value u_n to get

$$u' = J_n u + f_n(u)$$

  with $\qquad J_n = Df(u_n), \quad f_n(u) = F(u) - J_n u.$

- Apply an explicit exponential RK method

Hochbruck, O., Schweitzer (2006, 2009), Tokman (2006)

The exponential Rosenbrock–Euler method

Applying the exponential Euler method to

$$u' = F(u) = J_n u + f_n(u)$$

yields the exponential Rosenbrock–Euler method. It can be rewritten as

$$\begin{aligned} u_{n+1} &= \mathrm{e}^{h_n J_n} u_n + h_n \varphi_1(h_n J_n) f_n(u_n) \\ &= \mathrm{e}^{h_n J_n} u_n + h_n \varphi_1(h_n J_n) \big(F(u_n) - J_n u_n\big) \\ &= u_n + h_n \varphi_1(h_n J_n) F(u_n). \end{aligned}$$

Theorem. The exponential Rosenbrock–Euler method has order two.

Error analysis in a nutshell

Aim: comprehensive error analysis for stiff problems.

Basic assumptions:

- Temporal smoothness of the exact solution;
- Bounds on the (linear) evolution operators

$$\left\| \mathrm{e}^{tJ_n} \right\| \le C\, \mathrm{e}^{\omega t}, \qquad t \ge 0,$$

$$\left\| \mathrm{e}^{tJ_n} - \mathrm{e}^{tJ_{n-1}} \right\| \le C\, h_{n-1} \mathrm{e}^{\omega t}, \qquad t \ge 0.$$

Typically fulfilled for evolution equations in the framework of analytic semigroups.

Finite dimensional ODEs and parabolic problems.

Error analysis for the Rosenbrock–Euler method

We illustrate the main ideas for the exponential Rosenbrock–Euler method

$$u_{n+1} = \mathrm{e}^{h_n J_n} u_n + h_n \varphi_1(h_n J_n)\, f_n(u_n).$$

Inserting the exact solution into the numerical scheme gives

$$u(t_{n+1}) = \mathrm{e}^{h_n J_n} u(t_n) + h_n \varphi_1(h_n J_n)\, f_n\big(u(t_n)\big) - \delta_{n+1}$$

with defects $\|\delta_{n+1}\| \le C \cdot h^3$.

This implies the error recursion $E_n = u_n - u(t_n)$

$$E_{n+1} = \mathrm{e}^{h_n J_n} E_n + h_n \varphi_1(h_n J_n)\Big(f_n(u_n) - f_n\big(u(t_n)\big)\Big) + \delta_{n+1}.$$

Stability bound

The global errors $E_n = u_n - u(t_n)$ satisfy the recursion

$$E_{n+1} = \mathrm{e}^{h_n J_n} E_n + h_n \mathcal{N}_n(E_n) E_n + h_n^3 \mathcal{R}_{n+1}$$

with bounded operators $\mathcal{N}_n$ and bounded remainders $\mathcal{R}_{n+1}$.

Its stability is all-important.

Theorem. There exist constants C and Ω such that

$$\left\| \mathrm{e}^{h_n J_n} \cdots \mathrm{e}^{h_0 J_0} \right\| \;\leq\; C\,\mathrm{e}^{\Omega(h_0 + \ldots + h_n)},$$

as long as the numerical solution remains in a neighbourhood of the exact solution.

Proof of stability bound

Proof. Consider for $\widetilde{\omega} > \omega$ the equivalent norm

$$\|x\| \;\le\; |||x|||_n = \sup_{t\ge 0} \mathrm{e}^{-\widetilde{\omega}t}\|\mathrm{e}^{tJ_n}x\| \;\le\; C\|x\|$$

which satisfies

$$\begin{aligned} |||x|||_n &= \sup_{t\ge 0}\, \mathrm{e}^{-\widetilde{\omega}t}\left\|\left(\mathrm{e}^{tJ_n} - \mathrm{e}^{tJ_{n-1}} + \mathrm{e}^{tJ_{n-1}}\right)x\right\| \\ &\le |||x|||_{n-1} + \sup_{t\ge 0}\, \mathrm{e}^{-\widetilde{\omega}t}\left\|\mathrm{e}^{tJ_n} - \mathrm{e}^{tJ_{n-1}}\right\|\,\|x\| \\ &\le \left(1 + Ch_{n-1}\right)|||x|||_{n-1}, \qquad n \ge 1. \end{aligned}$$

Thus $\quad |||\mathrm{e}^{h_nJ_n}y|||_n \le \mathrm{e}^{\widetilde{\omega}h_n}|||y|||_n \le \mathrm{e}^{\widetilde{\omega}h_n}\mathrm{e}^{Ch_{n-1}}|||y|||_{n-1},$

where $y = \mathrm{e}^{h_{n-1}J_{n-1}}\cdots\mathrm{e}^{h_0J_0}u$.

Order conditions

order	order condition
1	$\sum_{i=1}^{s} b_i(hJ) = \varphi_1(hJ)$
2	$\sum_{j=1}^{i-1} a_{ij}(hJ) = c_i\varphi_1(c_i hJ), \quad 2 \le i \le s$
3	$\sum_{i=2}^{s} b_i(hJ)c_i^2 = 2\varphi_3(hJ)$
4	$\sum_{i=2}^{s} b_i(hJ)c_i^3 = 6\varphi_4(hJ)$

Order conditions for exponential Rosenbrock-type methods up to order 4.

Embedded methods of order 3 and 4

erow32: Third-order method with second-order error est.

$$
\begin{array}{c|cc}
c_2 & a_{21} & \\
\hline
 & b_1 & b_2 \\
 & \widehat{b}_1 &
\end{array}
\quad = \quad
\begin{array}{c|cc}
1 & \varphi_1 & \\
\hline
 & \varphi_1 - 2\varphi_3 & 2\varphi_3 \\
 & \varphi_1 &
\end{array}
$$

erow43: Fourth-order method with third-order error est.

$$
\begin{array}{c|ccc}
\frac{1}{2} & \frac{1}{2}\varphi_1\left(\frac{1}{2}\,\cdot\right) & & \\
1 & 0 & \varphi_1 & \\
\hline
 & \varphi_1 - 14\varphi_3 + 36\varphi_4 & 16\varphi_3 - 48\varphi_4 & -2\varphi_3 + 12\varphi_4 \\
 & \varphi_1 - 14\varphi_3 & 16\varphi_3 & -2\varphi_3
\end{array}
$$

Outline

Computation of $\exp(hA)v$ and $\varphi(hA)v$

Exponential integrators require approximations to $\exp(hA)v$.

Our approach is based on interpolation methods.

- Approximate $\exp(hA)v$ by an interpolation polynomial; involves only matrix-vector multiplications.
- Sensitivity of the interpolation polynomial strongly depends on the interpolation nodes.
- Real Leja points are an attractive choice (Leja 1957, Reichel 1990)
  - distributed in a similar way as Chebyshev points;
  - defined recursively - goes well with Newton interpolation;
  - superlinear convergence.

parabolic problems: (Bergamaschi, Caliari, Martínez, Vianello)

Reformulation of the method

To approximate the products with the matrix functions efficiently, rewrite the vectors $f_n(U_{nj}) = F(U_{nj}) - J_n U_{nj}$ as

$$f_n(U_{nj}) = F(u_n) - J_n u_n + D_{nj},$$

where

$$D_{nj} = F(U_{nj}) - F(u_n) - J_n\big(U_{nj} - u_n\big).$$

Due to the simplifying assumption, the method is equivalent to

$$U_{ni} = u_n + c_i h_n \varphi_1(c_i h_n J_n) F(u_n) + h_n \sum_{j=1}^{i-1} a_{ij}(h_n J_n) D_{nj},$$

$$u_{n+1} = u_n + h_n \varphi_1(h_n J_n) F(u_n) + h_n \sum_{i=1}^{s} b_i(h_n J_n) D_{ni}.$$

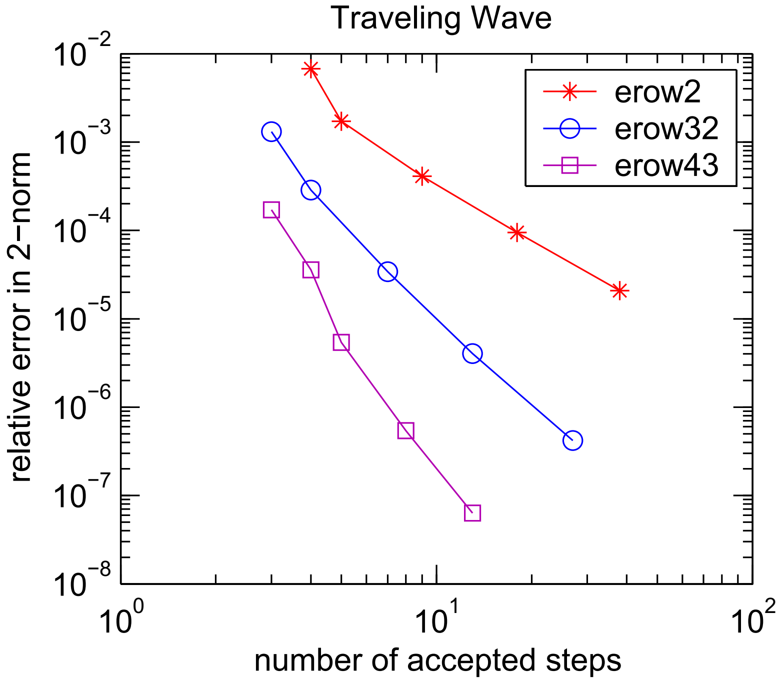
Note that $\|D_{nj}\| = O(h_n^2)$.

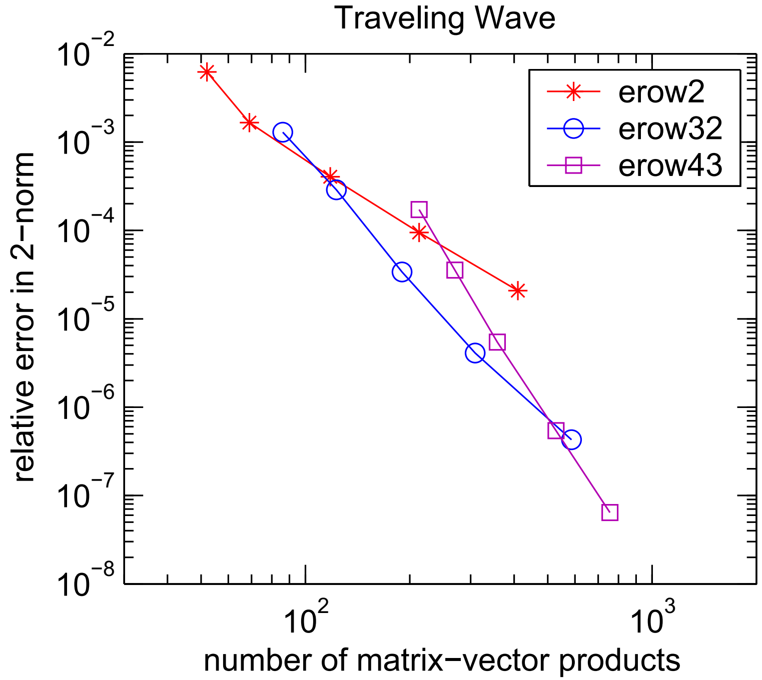
Example: reaction-diffusion-advection equation

Consider for $(x, y) \in [0,1]^2$ and $0 \le t \le 0.3$

$$\partial_t u = \tfrac{1}{20}(\partial_{xx} u + \partial_{yy} u) + \partial_x u + \partial_y u + u(u - \tfrac{1}{2})(1 - u)$$

smooth initial pulse, homogeneous Neumann b.c.
standard finite differences in space: $\Delta x = \Delta y = 0.05$





Outline

Application: exponential meshless method

Consider PDE

$$\partial_t u(t, \mathbf{x}) = Lu(t, \mathbf{x})$$

with L a second order, linear operator. Represent solution by interpolation

$$u(t, \mathbf{x}) \approx \sum_{j=1}^{N} \varphi_j(\mathbf{x}) U(t; \mathbf{x}_j) = \varphi(\mathbf{x}) \circ U(t)$$

where $\varphi_j(\mathbf{x}_i) = \delta_{ij}$ and collocate at the nodes $\{\mathbf{x}_i\}$ to get

$$U'(t) \; = \; AU(t), \qquad A_{ij} = L(\varphi_j)(\mathbf{x}_i), \quad A \in \mathbb{R}^{N\times N}$$

We solve this problem by an exponential integrator and approximate $\exp(h_n A) U_n$ by interpolation; requires tool to compute AV directly as $L\left(\varphi(\mathbf{x}) \circ V\right)\big|_{[\mathbf{x}_1,\ldots,\mathbf{x}_N]^\mathsf{T}}$.

Interpolation and error monitor

2d code for interpolation of scattered data:

CShep2D (Renka)

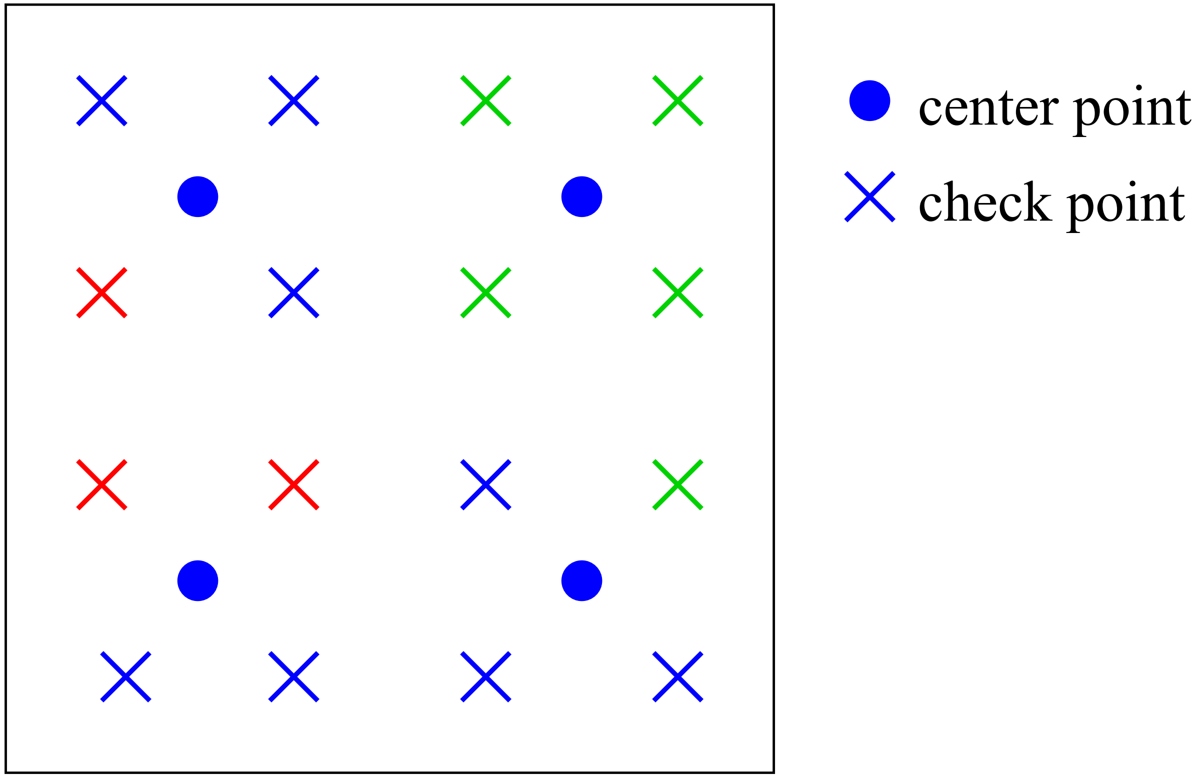
constructs a $\mathcal{C}^2$ interpolant in a moving least-square fashion.

Since the collocation, or center, points are arbitrary, we can add or remove points at each time step, depending on the behaviour of the solution on a set of check points.

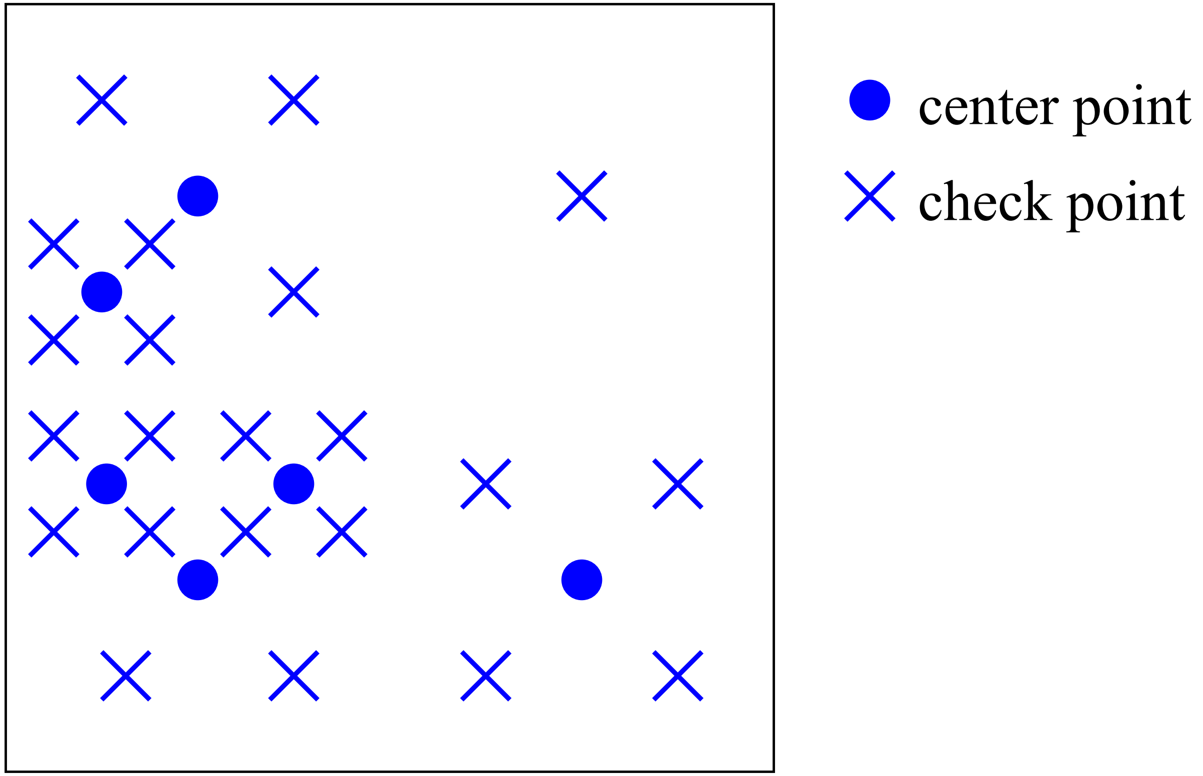
Error monitor: use a curvature monitor at each check point $\check{\mathbf{x}}_i$

$$|\Delta x^2 \partial_{xx} u(t; \check{\mathbf{x}}_i)| + |\Delta y^2 \partial_{yy} u(t; \check{\mathbf{x}}_i)|$$

Center and check points



Center and check points



The Molenkamp–Crowley test

Consider

$$\partial_t u \;=\; \partial_x(au) + \partial_y(bu)$$

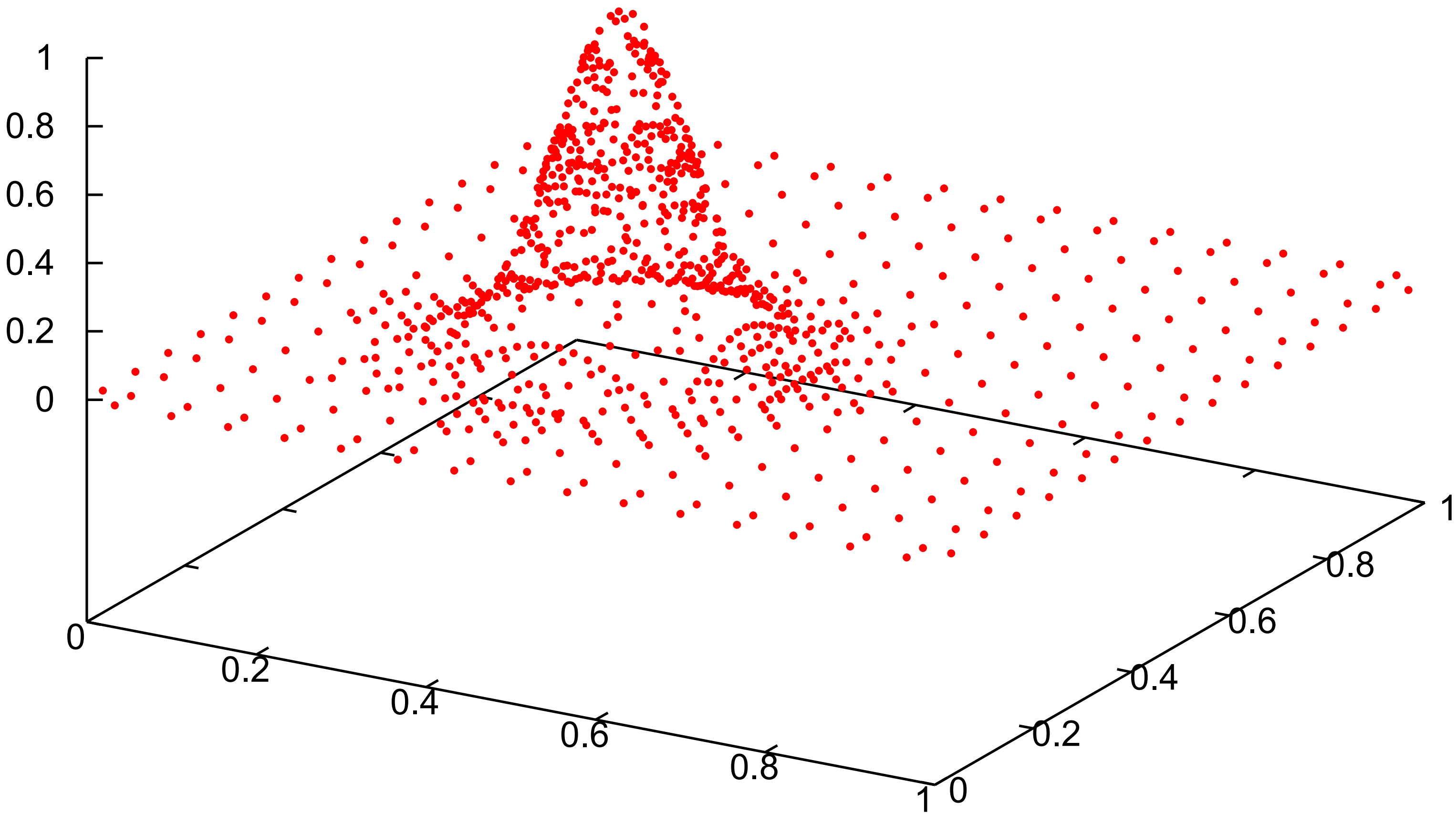
with

$$a(x,y) = 2\pi\left(y - \frac{1}{2}\right), \quad b(x,y) = -2\pi\left(x - \frac{1}{2}\right)$$

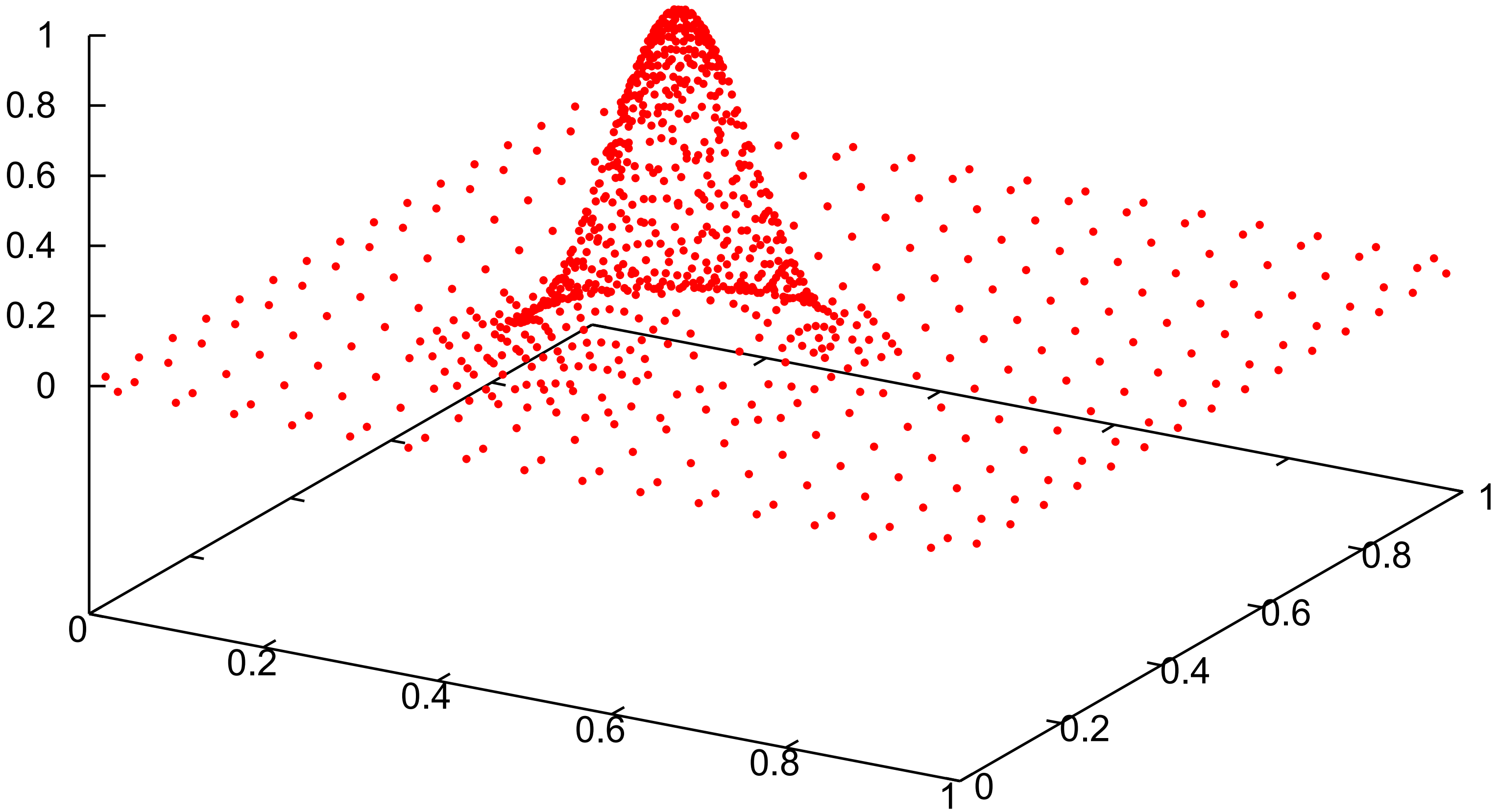
The initial profile is rotated around the center of the domain.

At time $t = 1$ one rotation will be completed. Homogeneous Dirichlet conditions are prescribed at inflow boundaries.

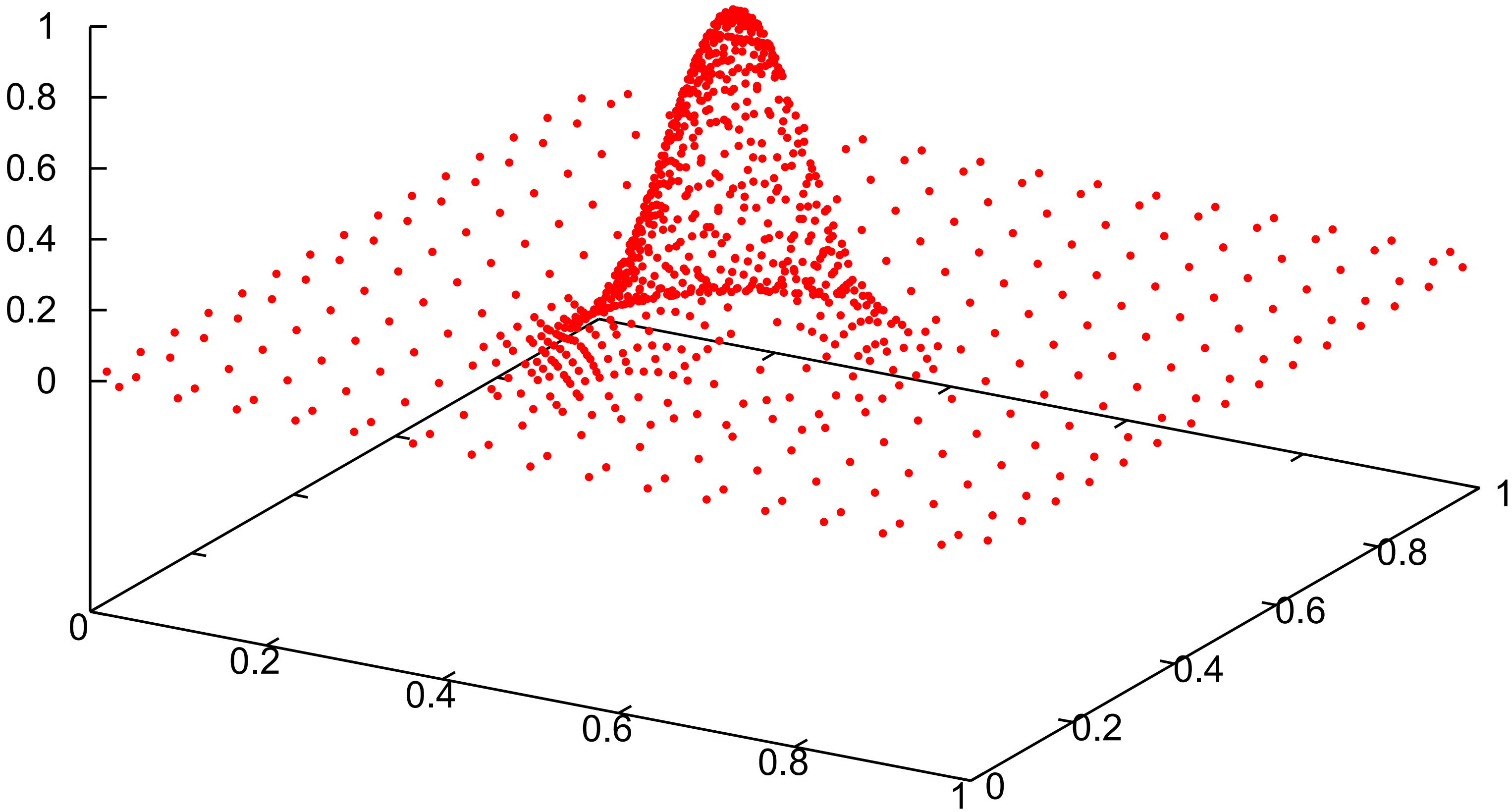
The Molenkamp–Crowley test



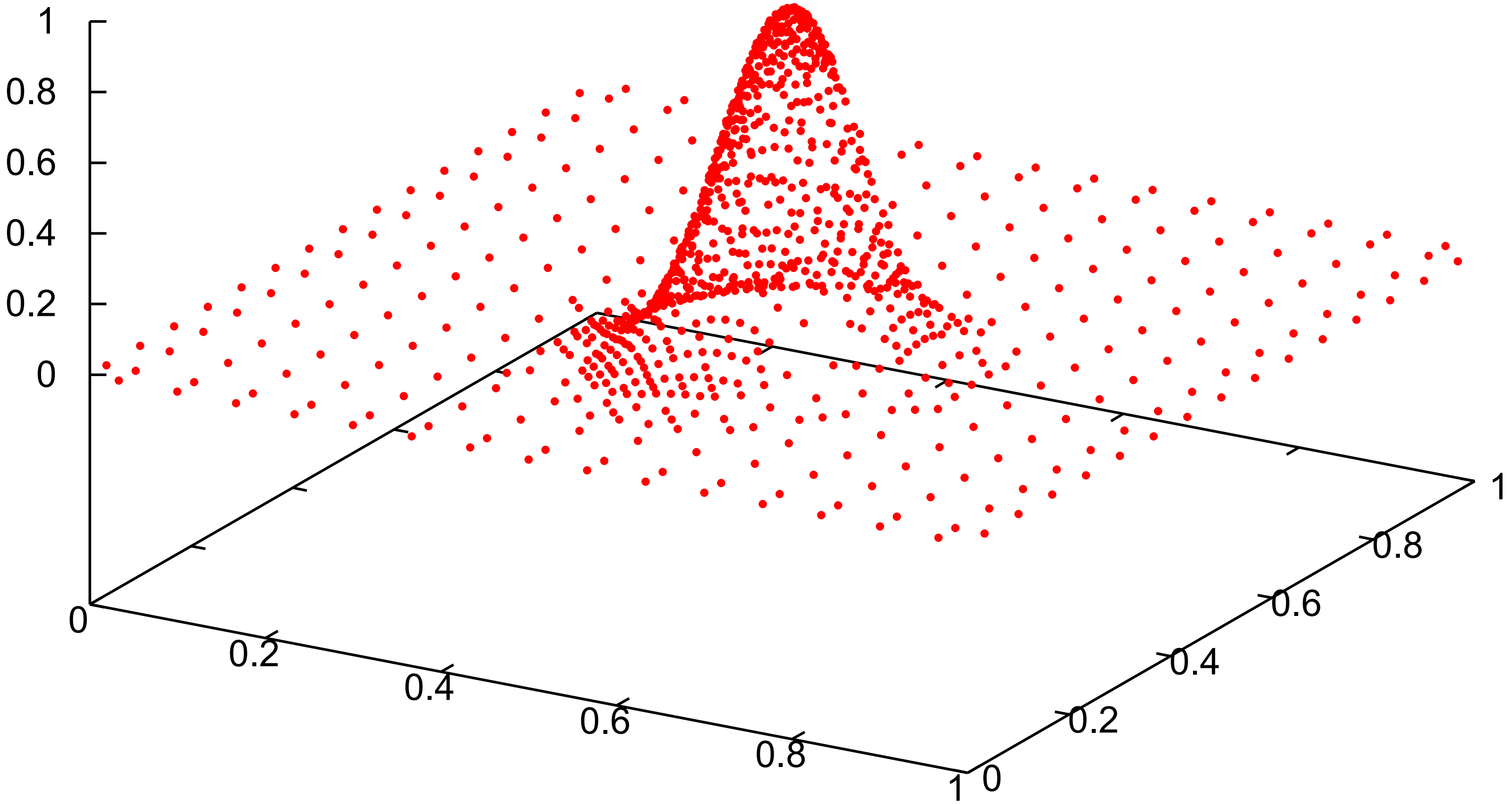
The Molenkamp–Crowley test



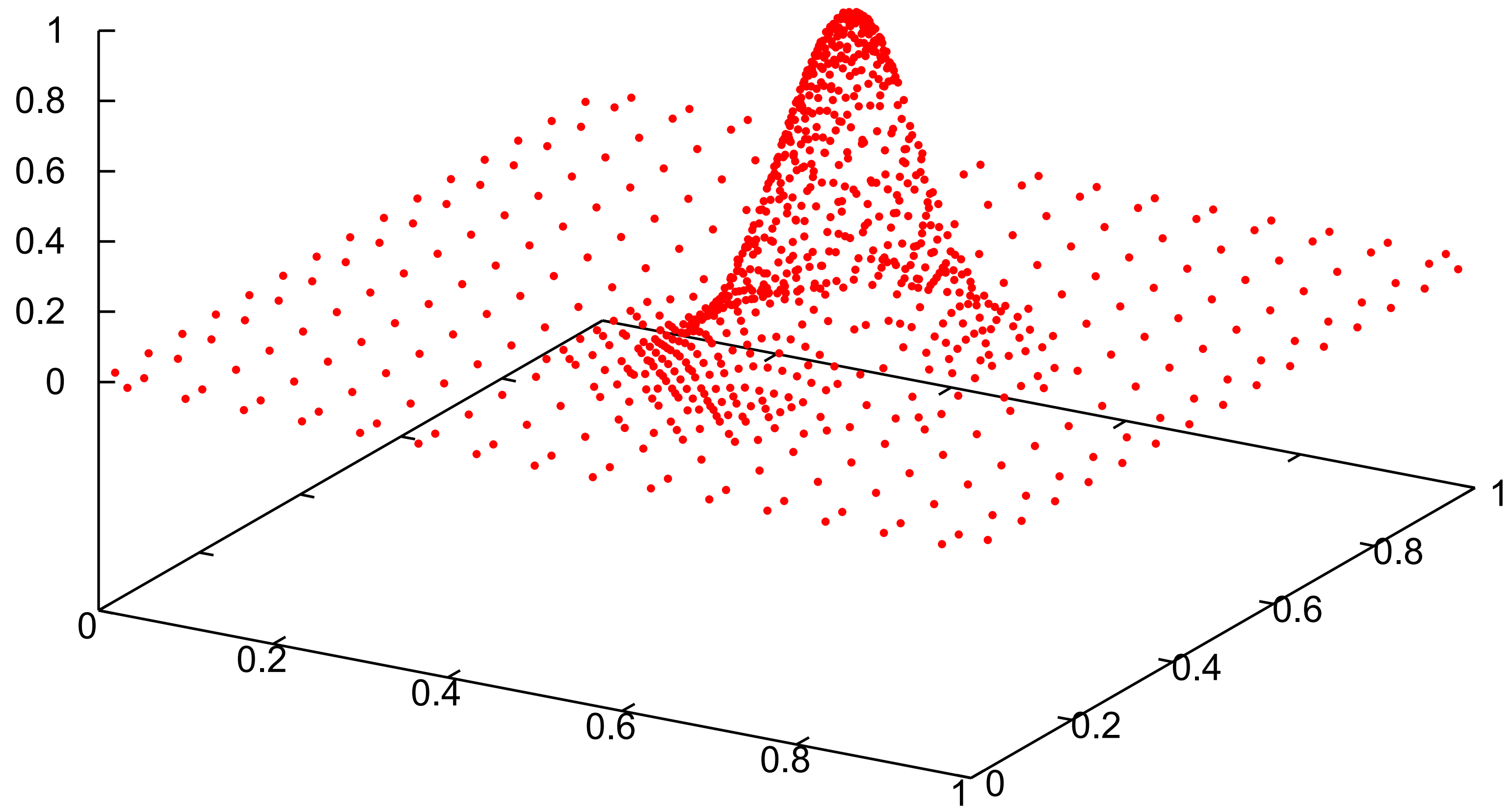
The Molenkamp–Crowley test



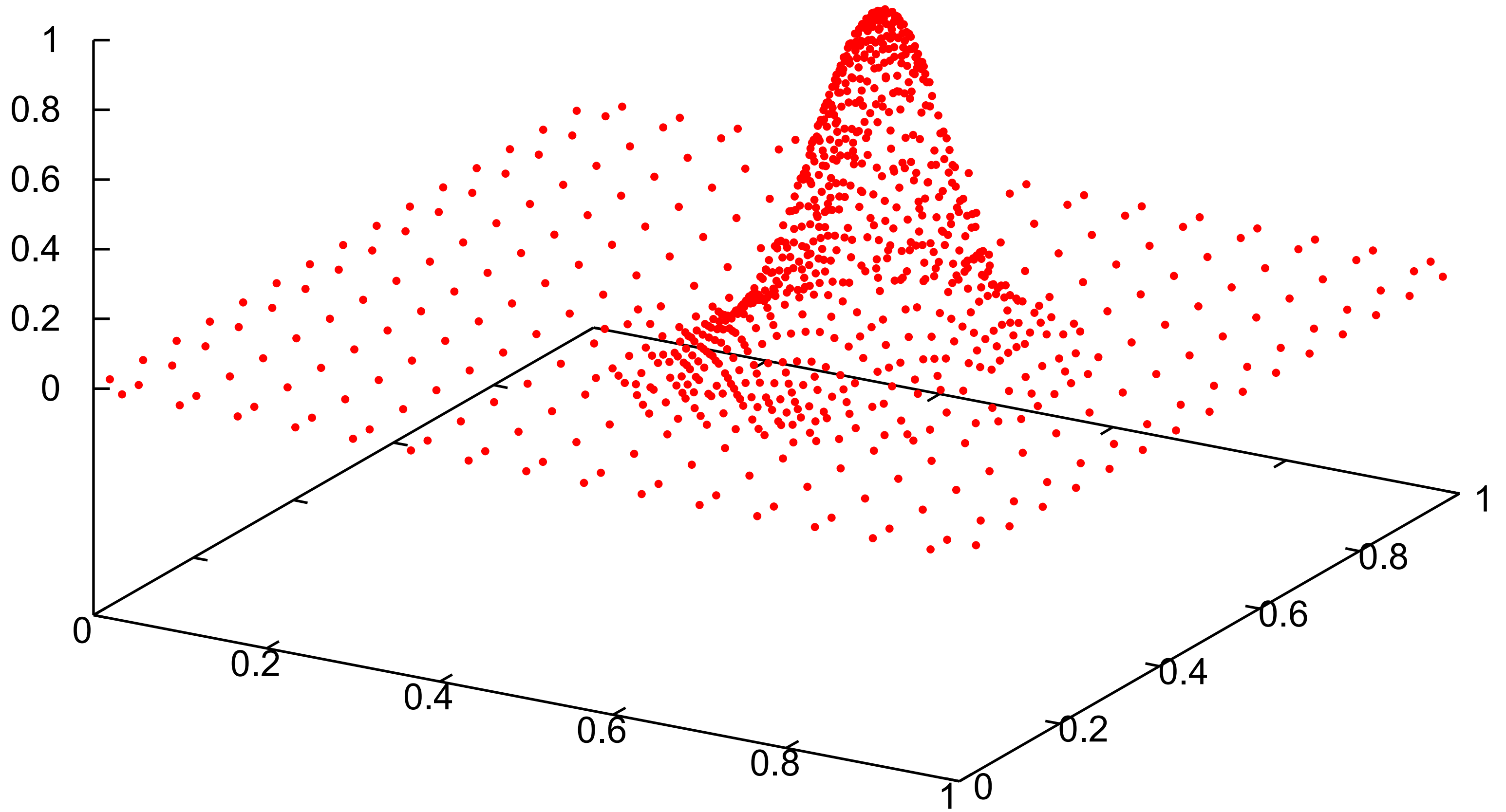
The Molenkamp–Crowley test



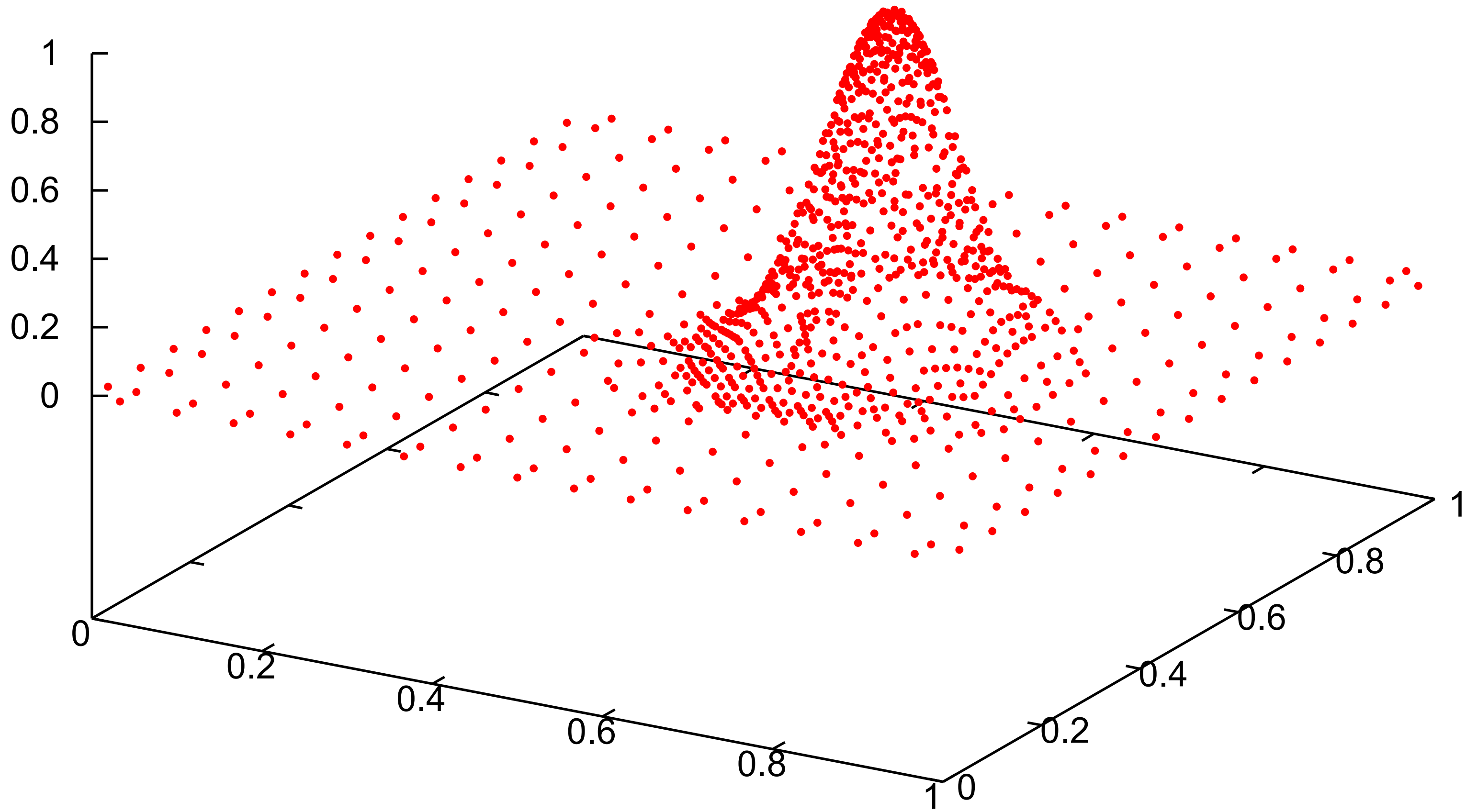
The Molenkamp–Crowley test



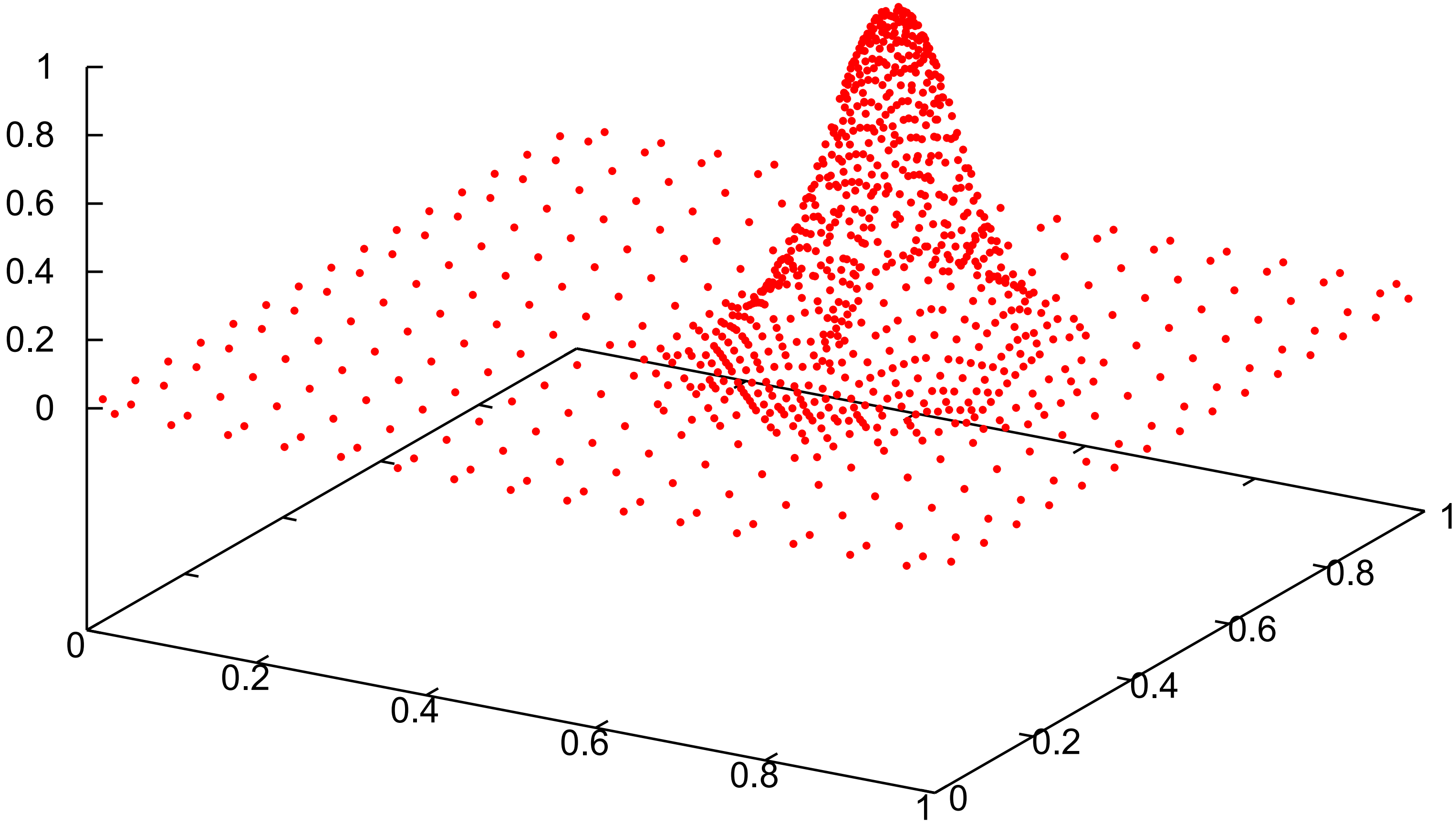
The Molenkamp–Crowley test



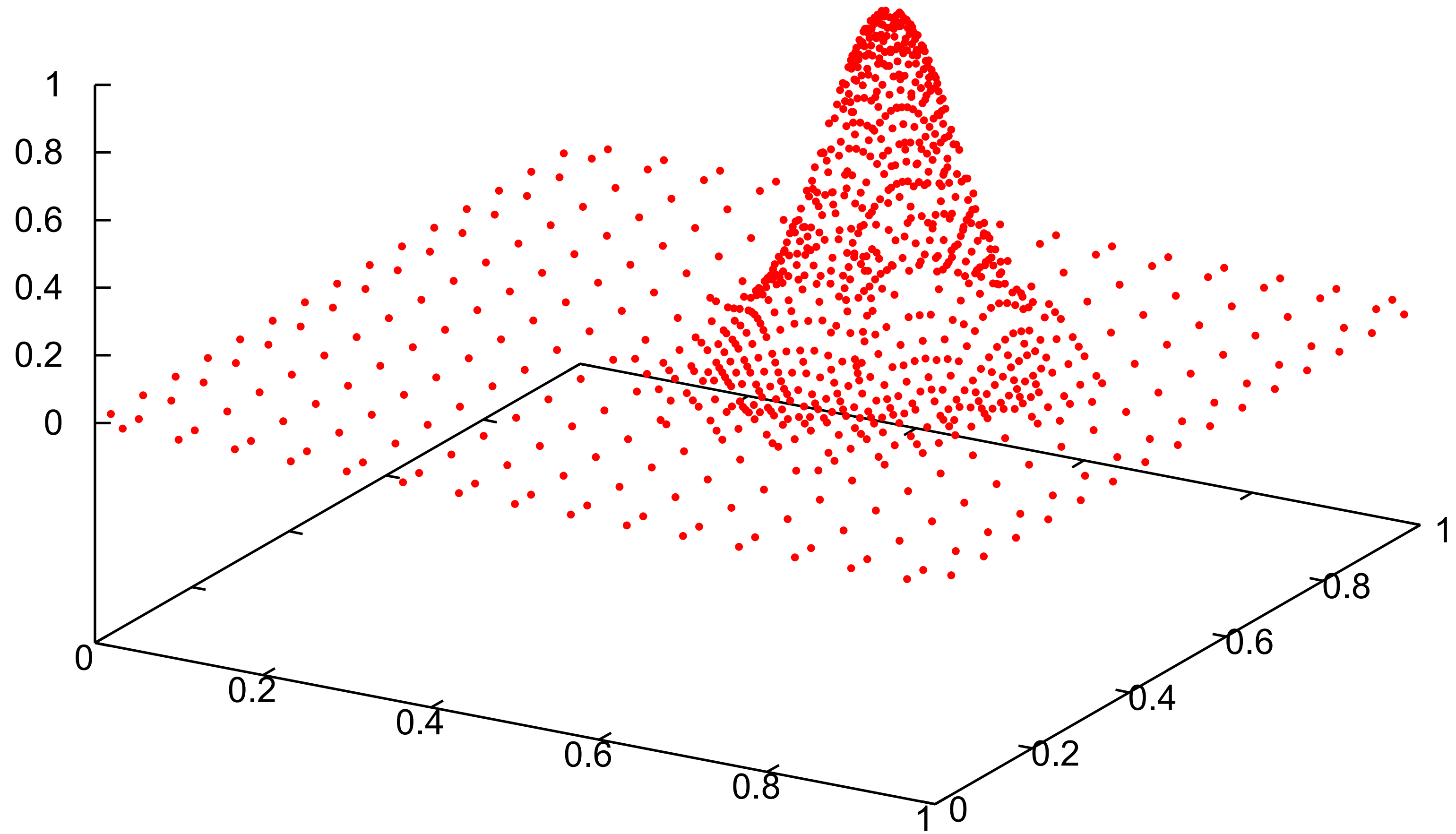
The Molenkamp–Crowley test



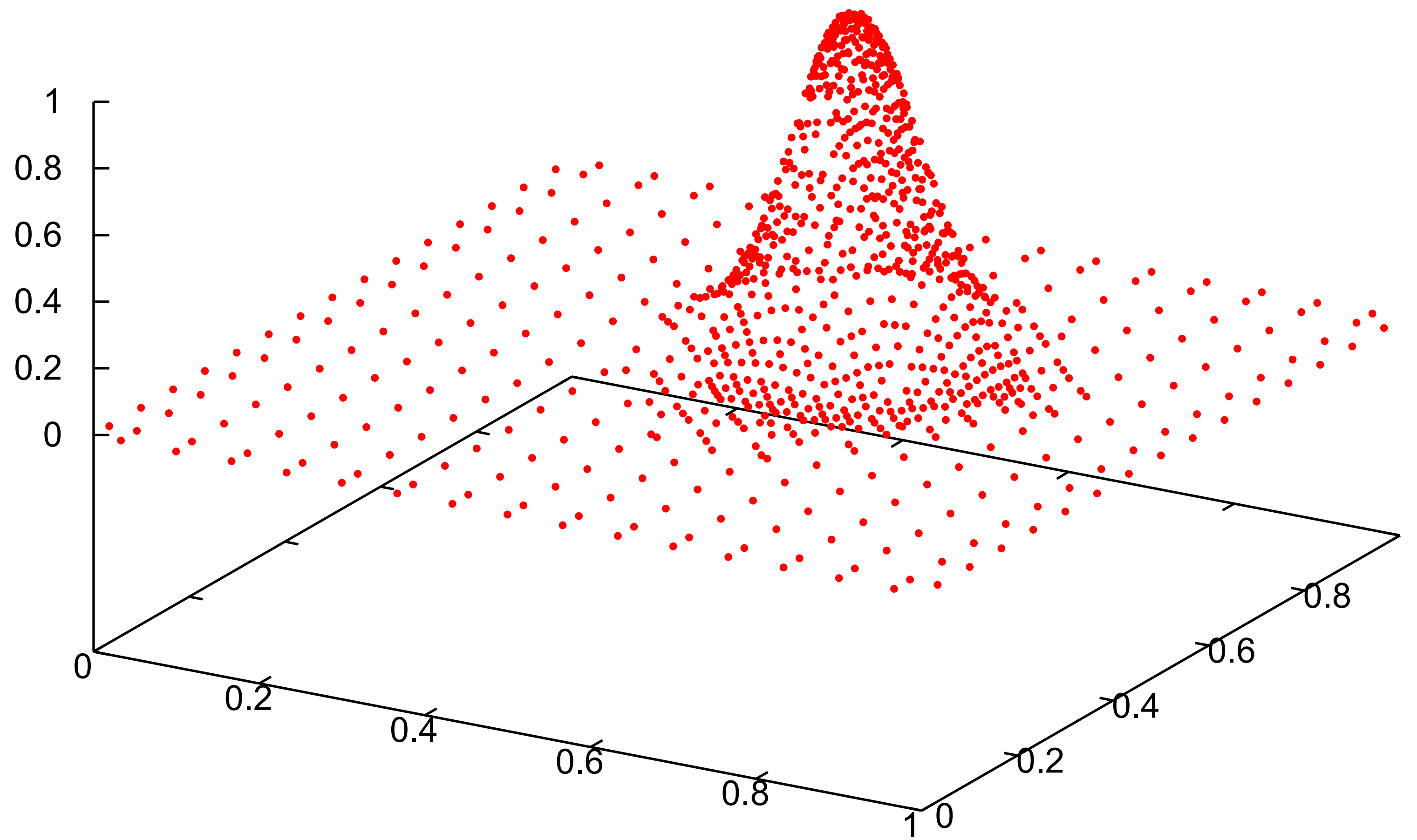
The Molenkamp–Crowley test



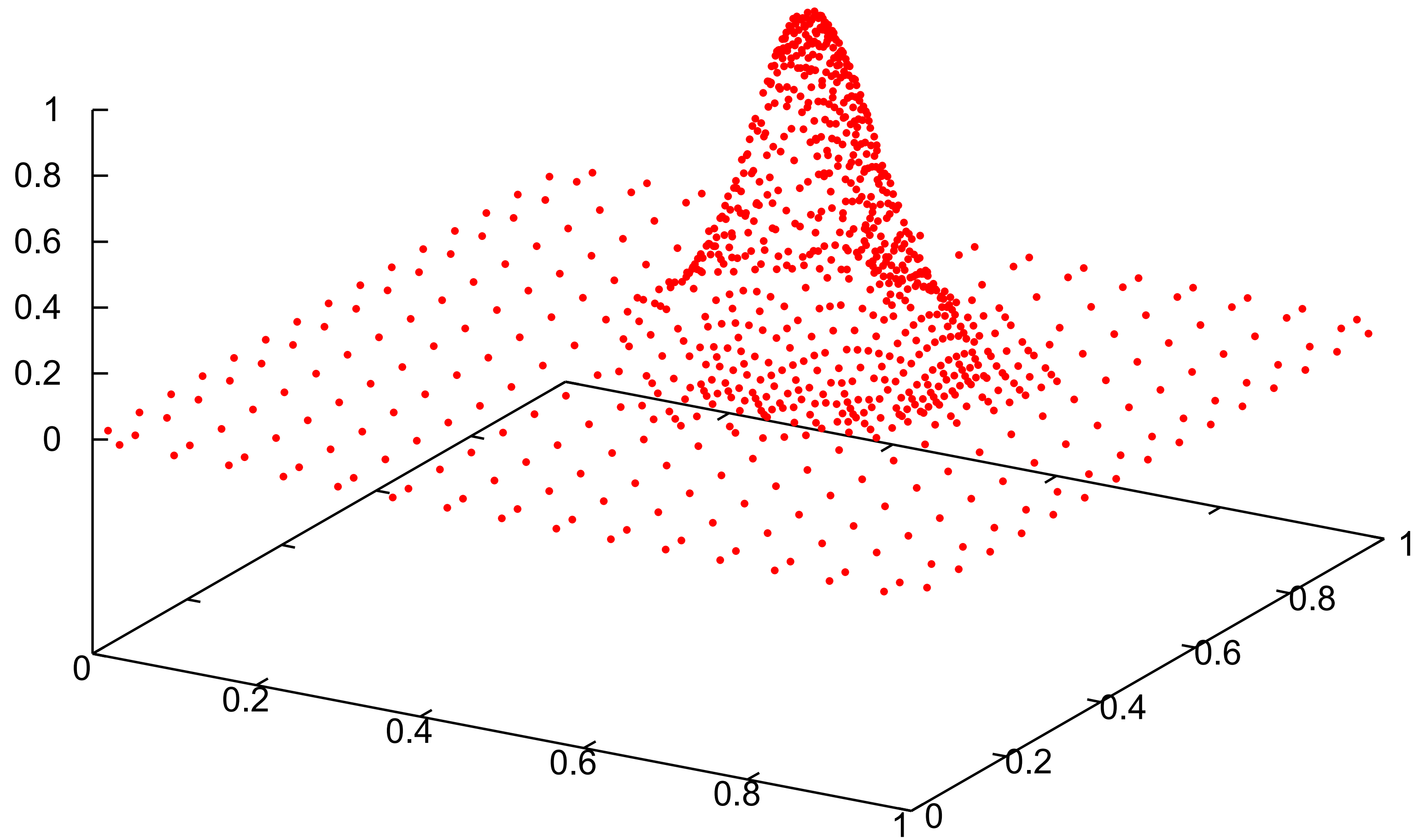
The Molenkamp–Crowley test



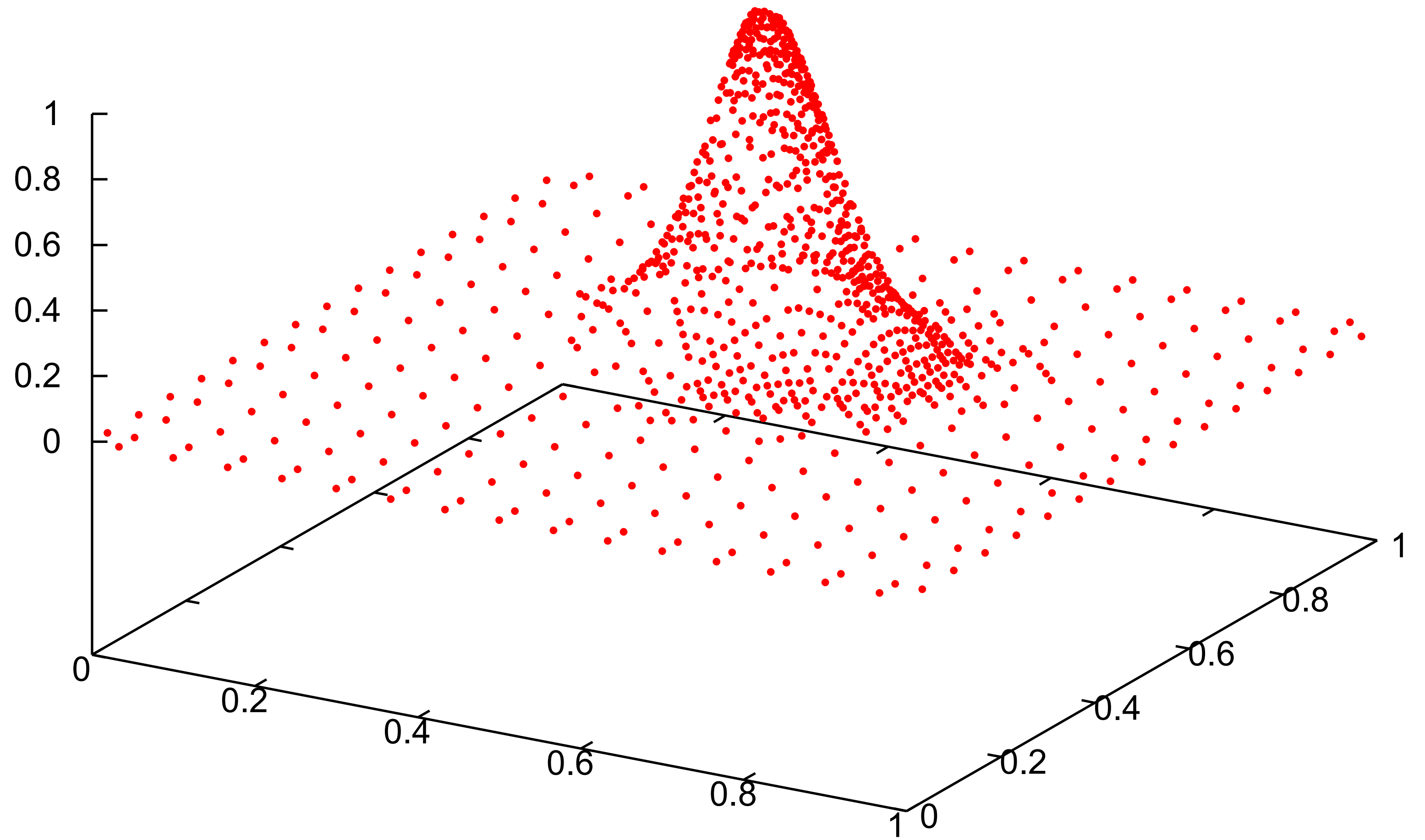
The Molenkamp–Crowley test



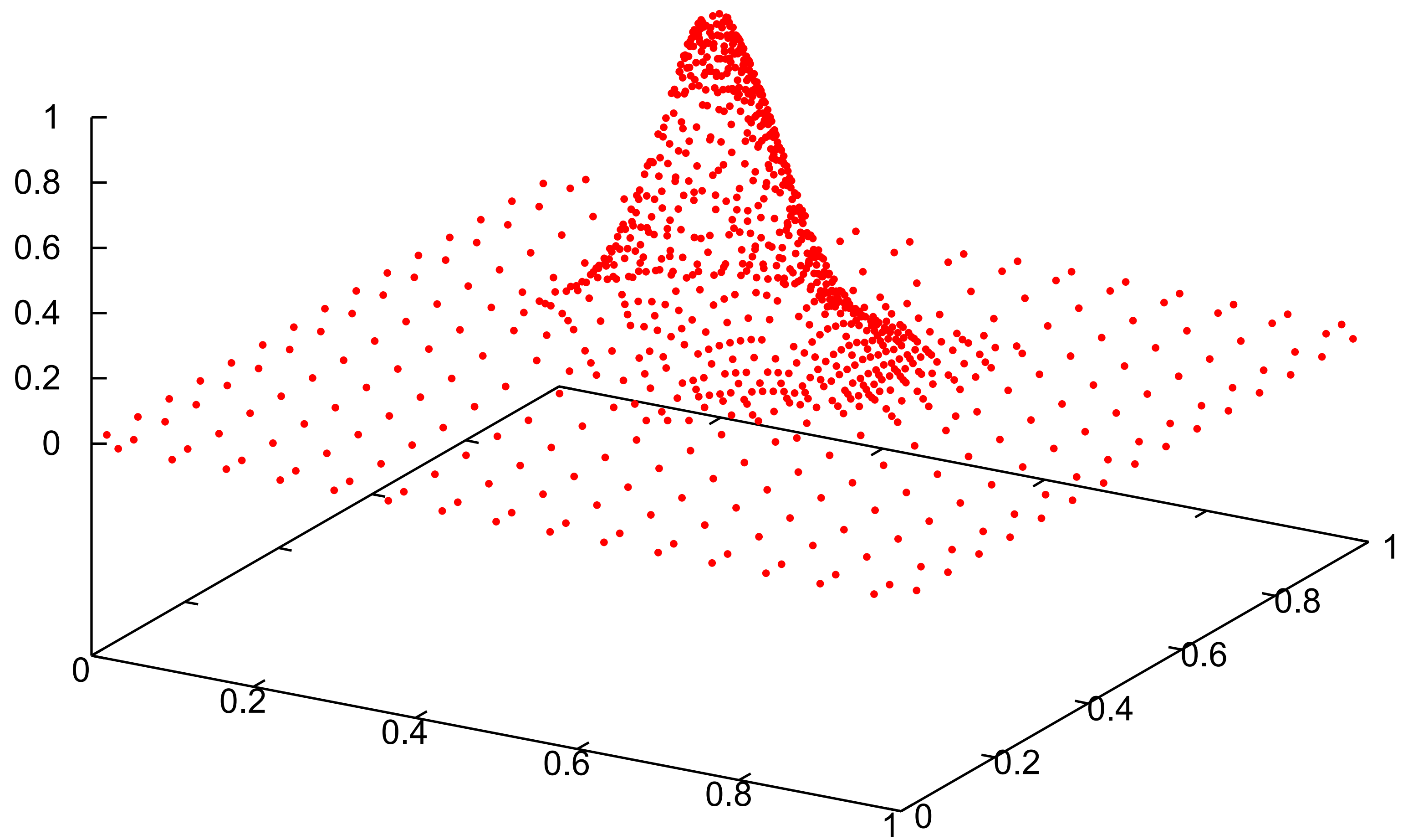
The Molenkamp–Crowley test



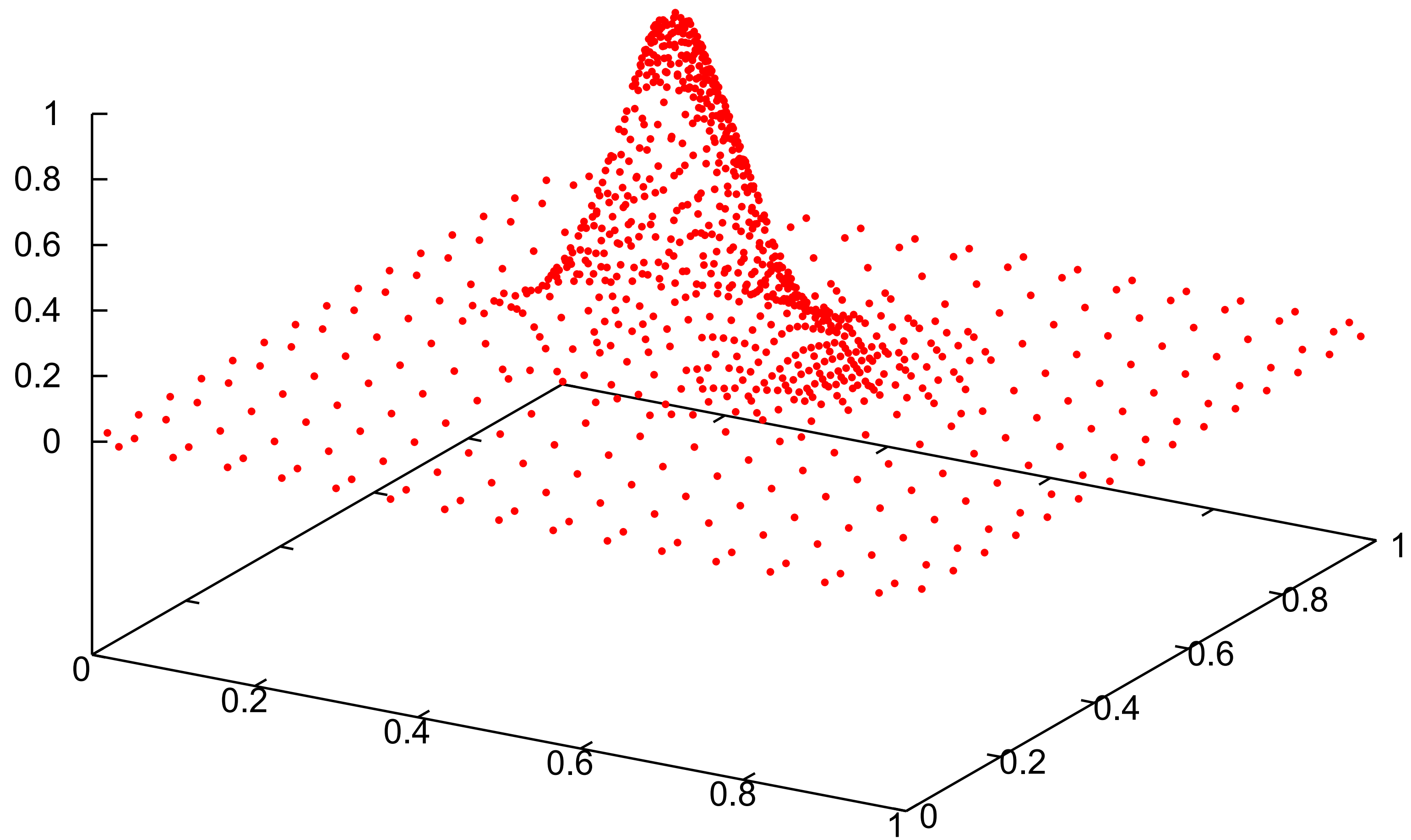
The Molenkamp–Crowley test



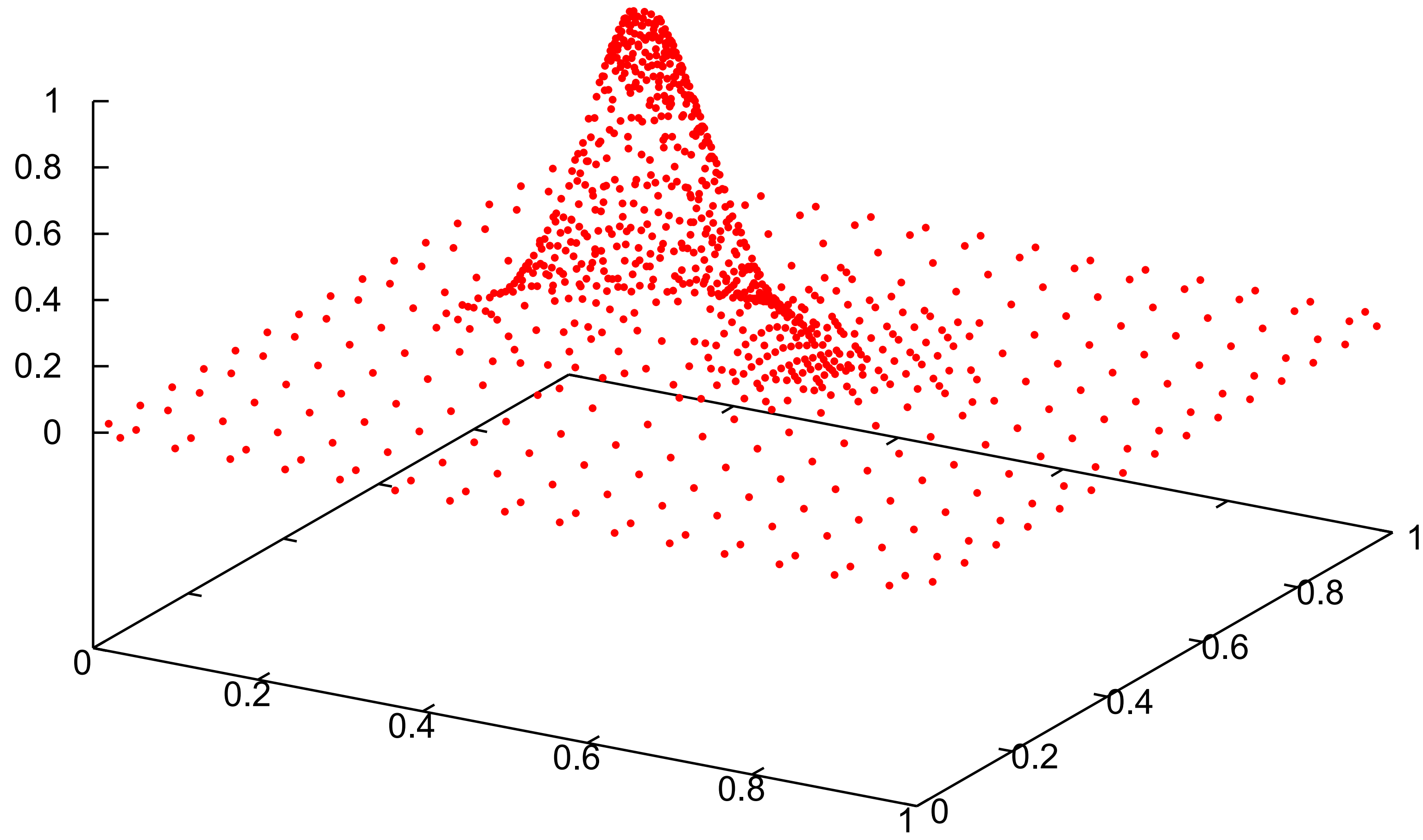
The Molenkamp–Crowley test



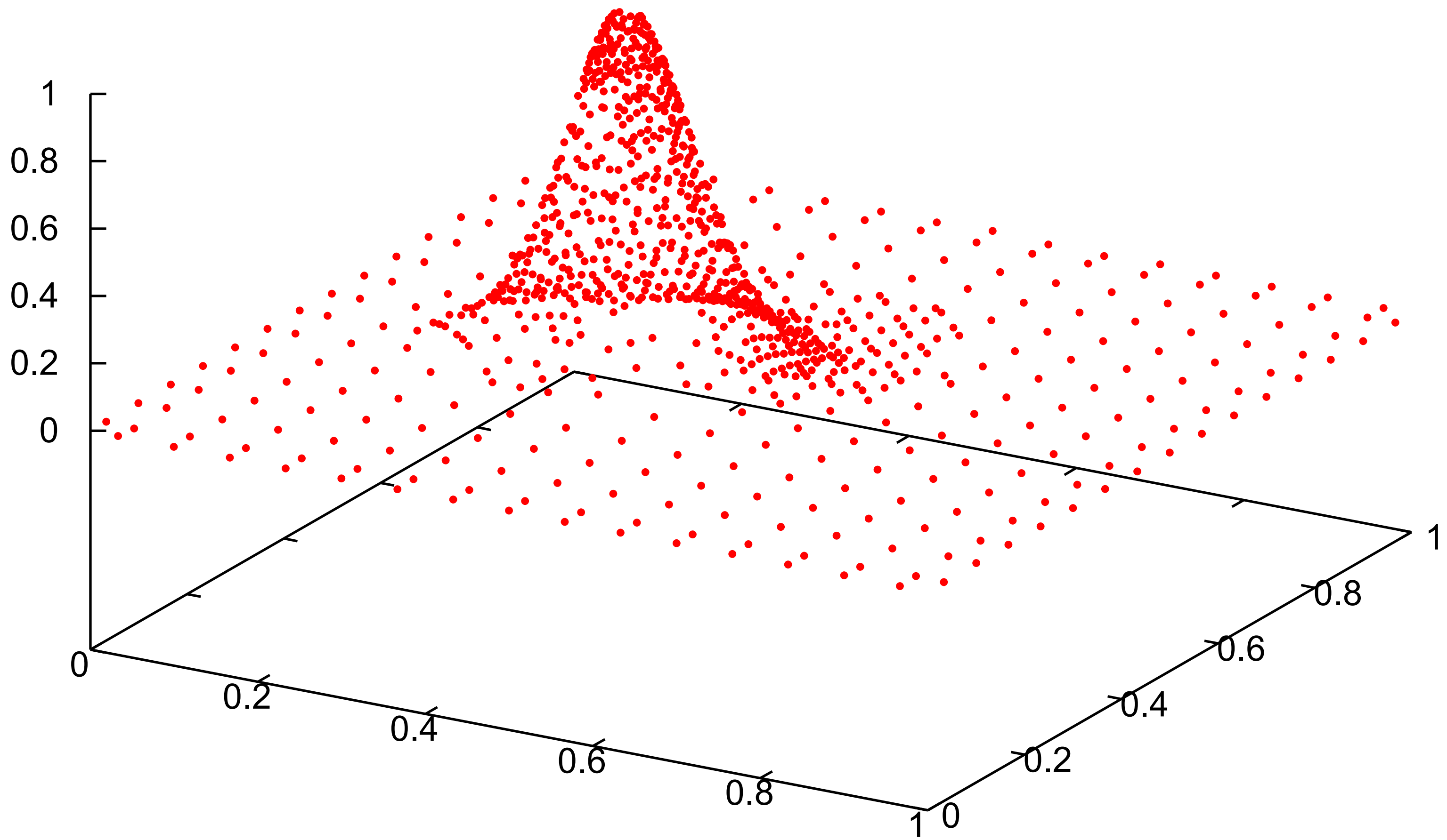
The Molenkamp–Crowley test



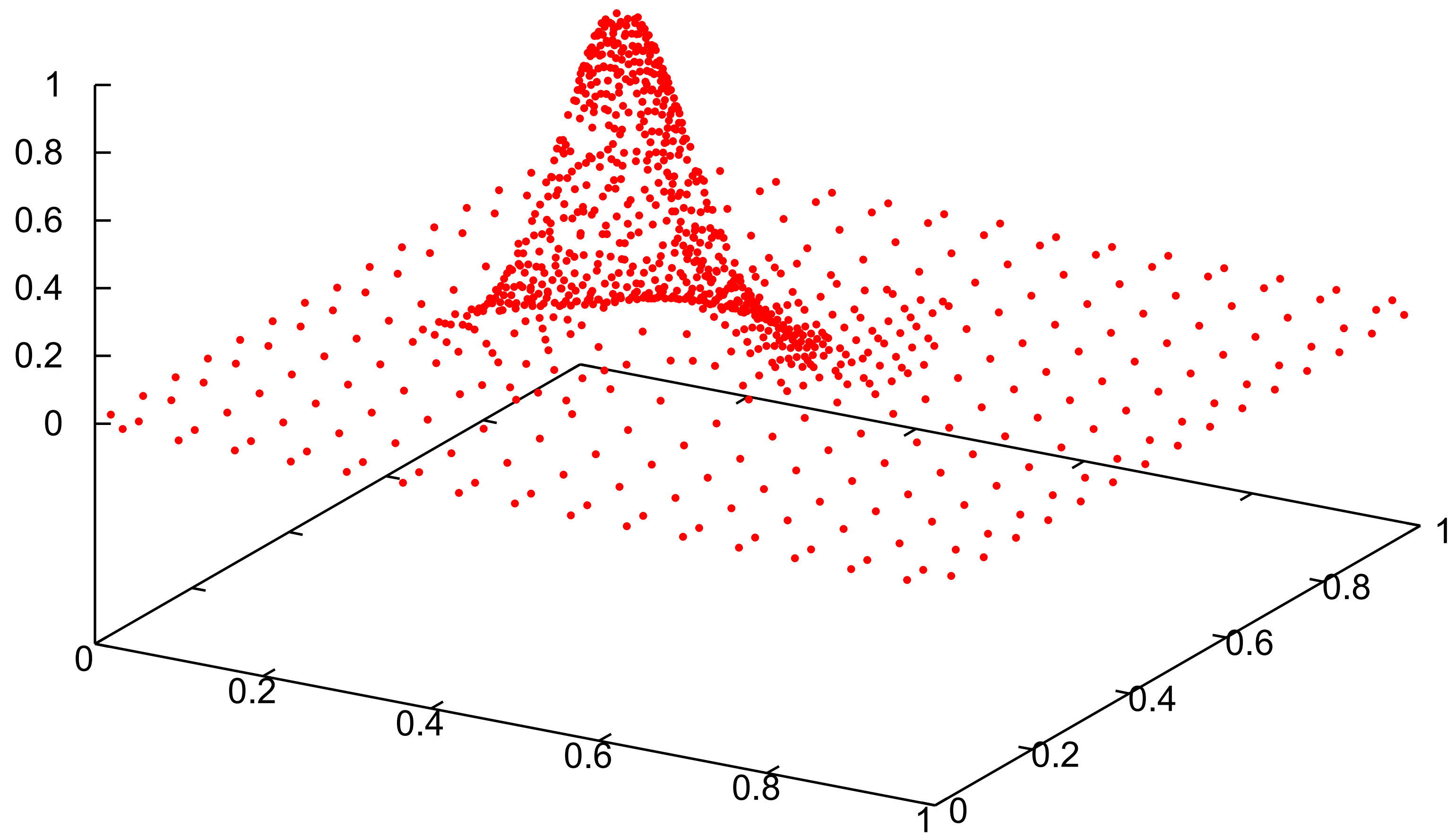
The Molenkamp–Crowley test



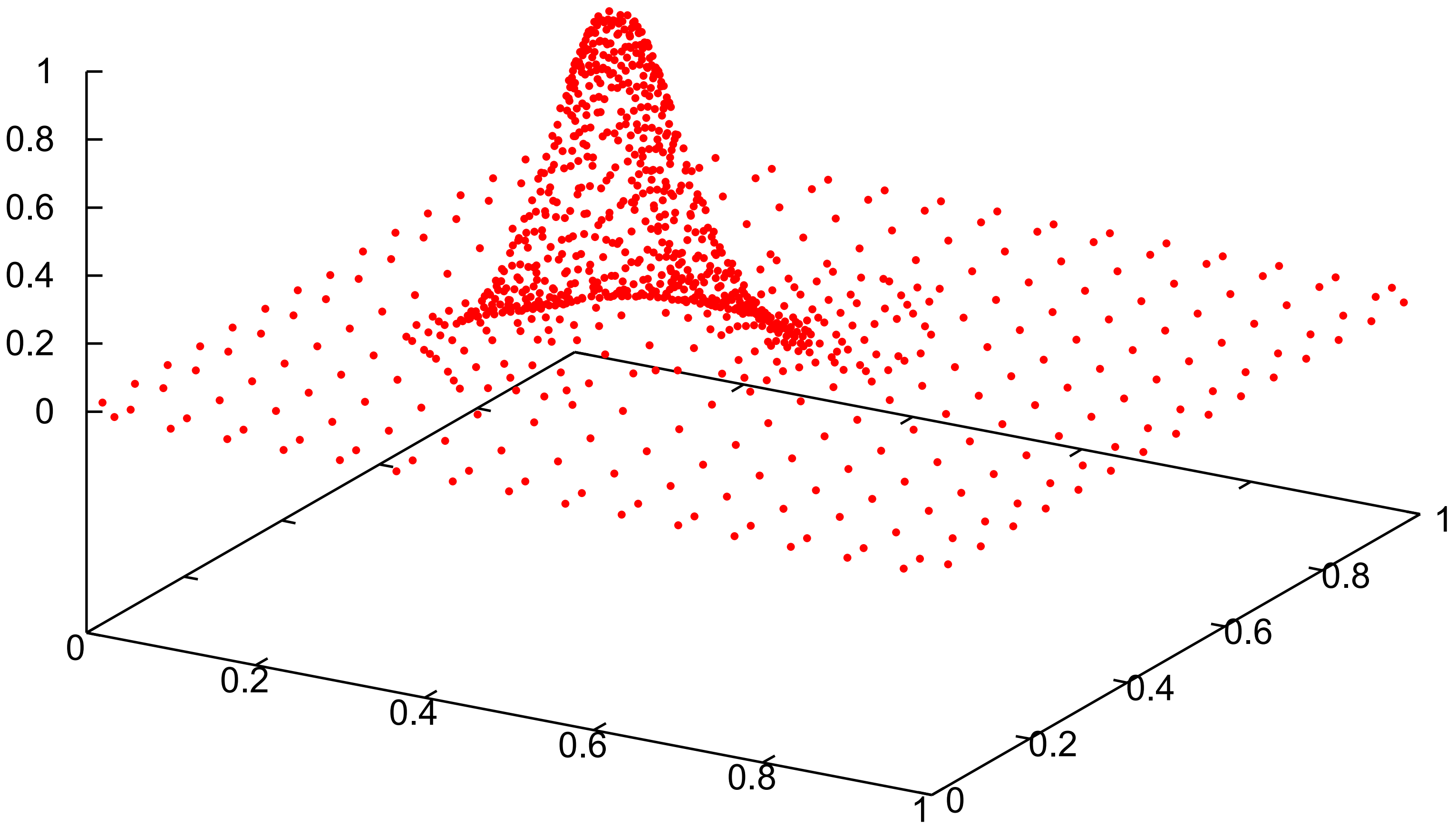
The Molenkamp–Crowley test



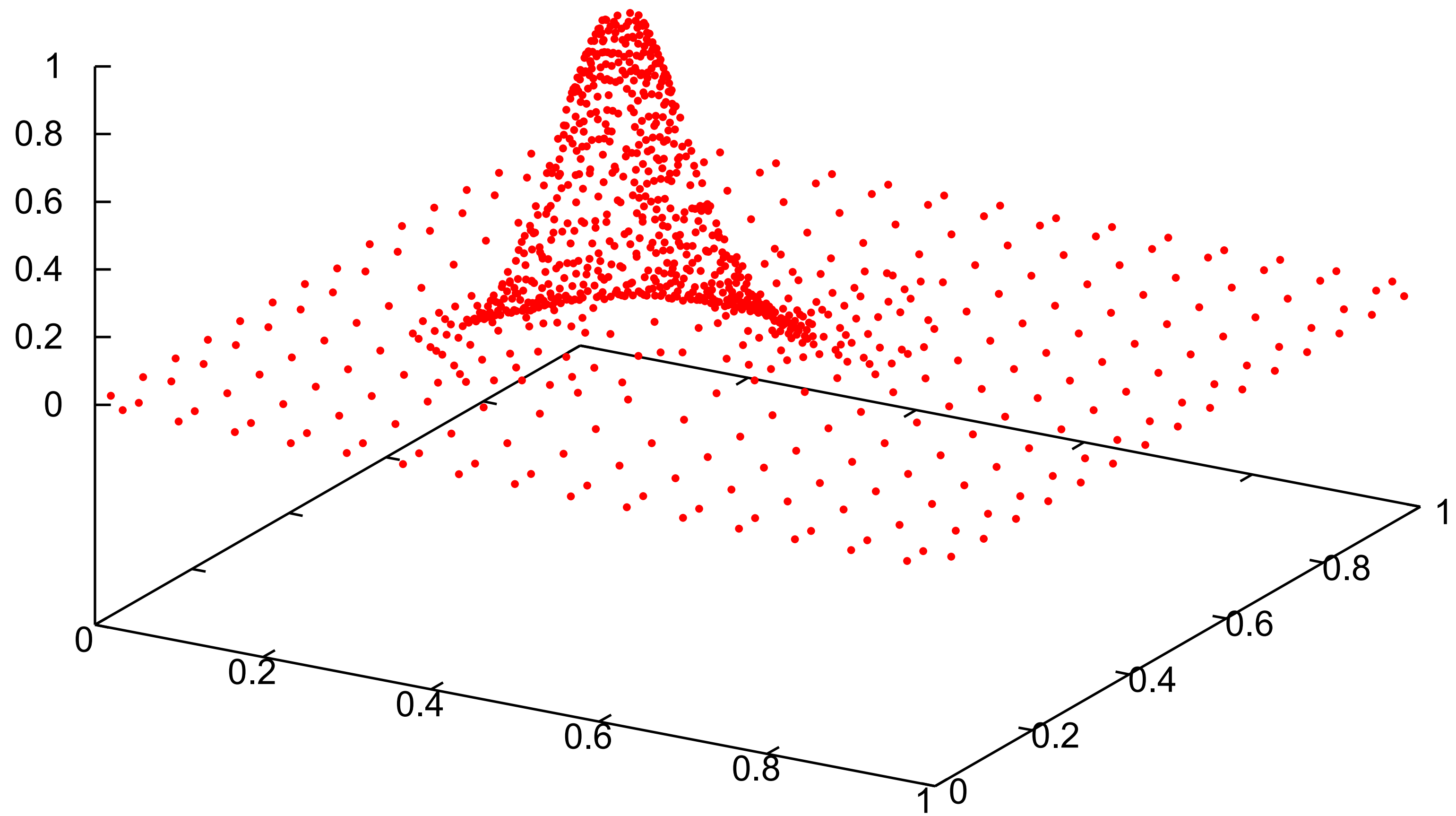
The Molenkamp–Crowley test



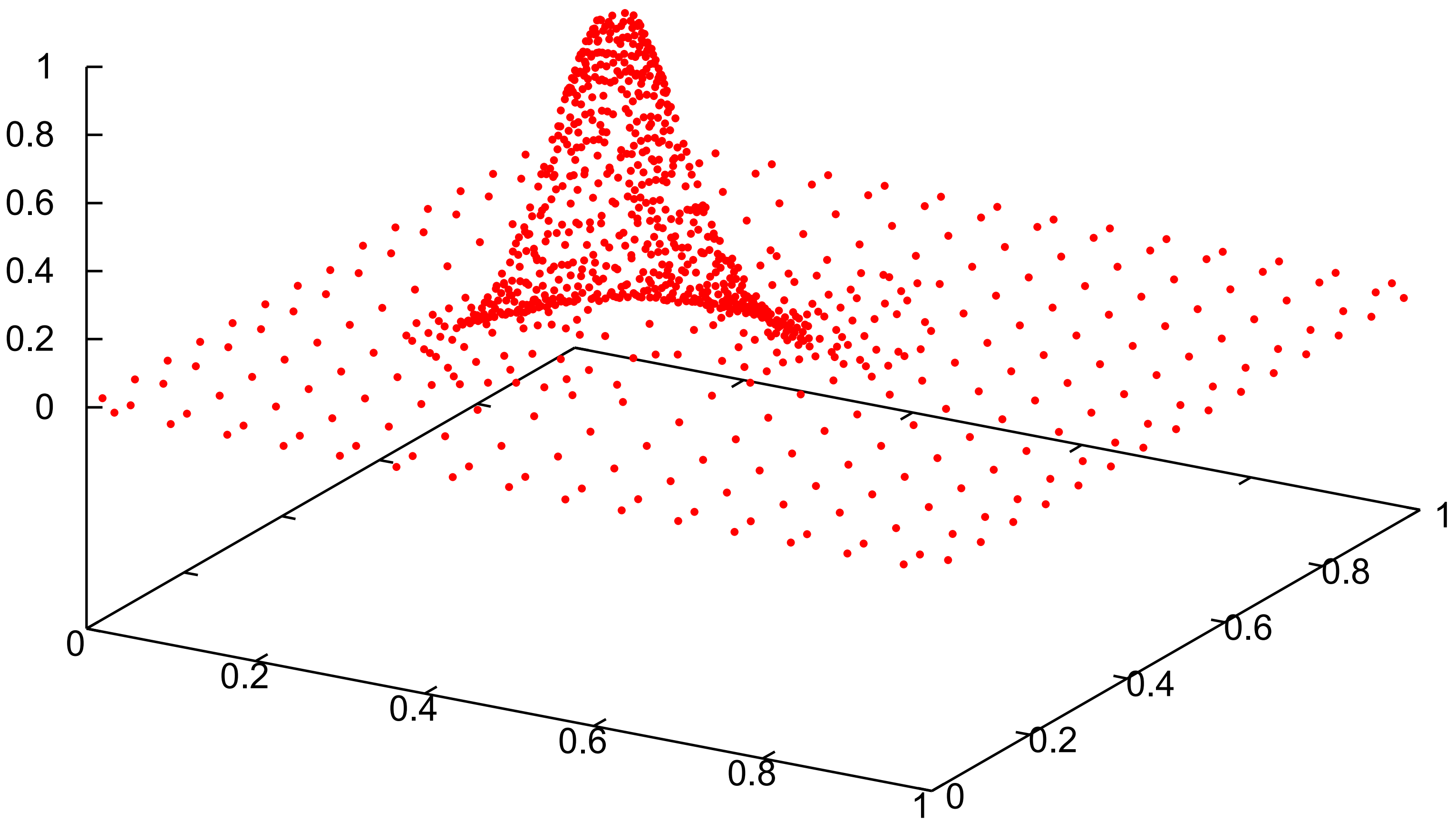
The Molenkamp–Crowley test



The Molenkamp–Crowley test



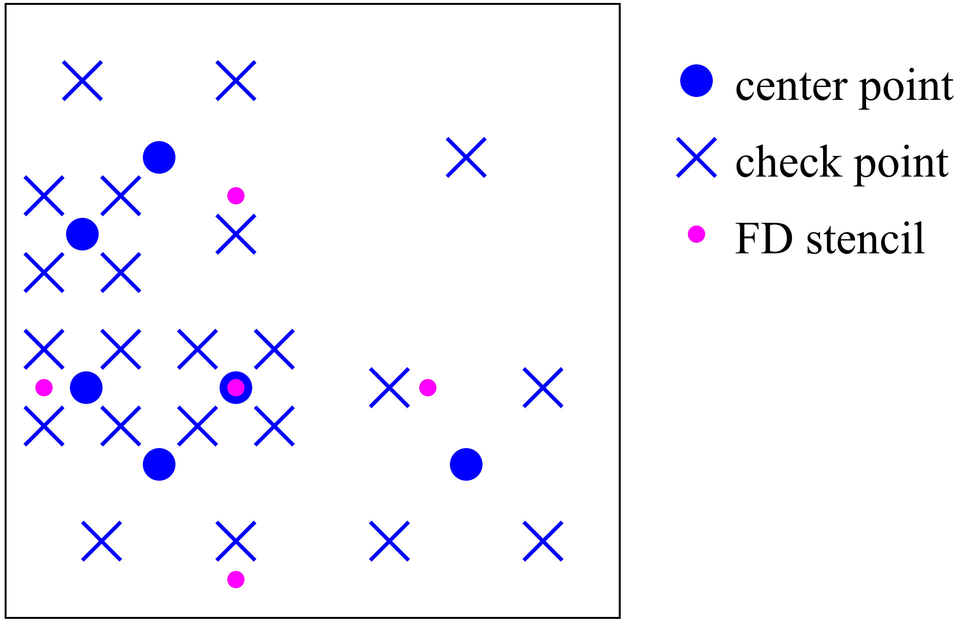
The Molenkamp–Crowley test



Unstable derivatives?

Derivatives computed directly by {C,Q}Shep2D give raise to small instabilities during time integration.

Numerical experiments show: derivatives, obtained by symmetric finite differences are much more stable.



Some references

M. Hochbruck, M. Hönig, A. Ostermann: A convergence analysis of the exponential Euler iteration for nonlinear ill-posed problems. To appear in Inverse Problems (2009)

M. Hochbruck, A. Ostermann, J. Schweitzer: Exponential Rosenbrock-type methods. SIAM J. Numer. Anal. 47, 786-803 (2009)

M. Caliari, A. Ostermann: Implementation of exponential Rosenbrock-type integrators. Applied Numerical Math. 59, 568-581 (2009)

A. Ostermann, M. Thalhammer, W. Wright: A class of explicit exponential general linear methods. BIT 46, 409-431 (2006)

M. Hochbruck, A. Ostermann: Explicit exponential Runge–Kutta methods for semilinear parabolic problems. SIAM J. Numer. Anal. 43, 1069-1090 (2005)

M. Hochbruck, A. Ostermann: Exponential Runge–Kutta methods for parabolic problems. Applied Numerical Math. 53, 323-339 (2005)