Meshfree integrators

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Geometric Numerical Integration

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Evolution equations

Consider time-dependent PDE

$$\frac{\partial}{\partial t}u(t,\xi) = F\Big(t,\xi,u(t,\xi),\frac{\partial}{\partial \xi}u(t,\xi),\ldots\Big)$$
$$t \in [0,T], \quad \xi \in \Omega \subset \mathbb{R}^d$$

subject to appropriate initial and boundary conditions.

Main assumption: The *essential support*

$$\{\xi \in \mathbb{R}^d \; ; \; |u(t,\xi)| \geq \varepsilon\}$$

is "small" and varying with time.

Meshfree integrator provides numerical solution

$$u_n(\xi) \approx u(t_n,\xi)$$

at discrete times $0 = t_0 < t_1 < t_2 < \ldots < t_N = T$.

Space discretization

Standard procedures:

- finite differences
- (moving) finite elements
- pseudospectal methods (e.g., in QM)
- ...

In this talk: meshfree methods
spatial function $f(\xi)$ is reconstructed by interpolation

Important issue: appropriate choice of basis functions

Compactly supported radial basis functions
Schaback, Wendland, Wu: several papers $\sim$ 1995
stationary problems

Space discretization – Wendland rbf

Interpolate $f : \mathbb{R}^d \to \mathbb{R}$ by radial basis functions

$$f(\xi) \approx s(\xi) = \sum_{\eta \in H} \lambda_\eta \Phi\big(\xi - \eta\big), \quad \Phi(\xi) = \psi(\|\xi\|)$$

using center points $H = \{\eta_1, \dots, \eta_m\}$. Our choice is

$$\psi(r) = (1 - r)_+^6 (35r^2 + 18r + 3)$$

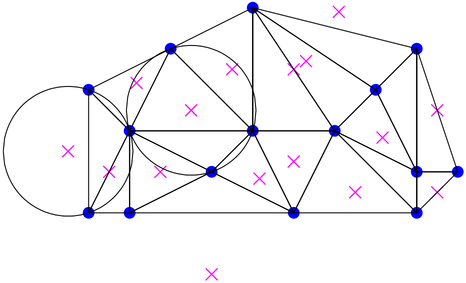
Coefficients λ_η are determined by interpolation matrix

$$B = \Big(\Phi\big(\eta_i - \eta_j\big)\Big)_{\{\eta_i, \eta_j\} \in H}$$

Positive definite (independently of the choice of points).

Center points (bullets) and check points (crosses)

Choose check points as circumcenters of a Delaunay triangulation of the center points.



- Check points maximize the local error bound.
- Adding such a check point as a new center point minimizes the growth of the condition number of interpolation matrix.
- Adding new points is simple.

Principles of a meshfree integrator

Residual subsampling

* Choose a set of candidate interpolation points

REPEAT

  * Interpolate the current solution $u_n(\xi)$ with respect to the actual set of candidate interpolation points
  * Check error and add/remove points using the thresholds θ_r, θ_c
  * Update the set of candidate interpolation points

UNTIL the set of candidate points remains fixed

* Take this set for the time step

Principles of a meshfree integrator, cont.

A single time step

* Start with set of candidate points

REPEAT

  * Compute the check points
  * Evaluate the current solution at the set of integration points (center and check pts.)
  * Perform the time step and control the error (both, temporal and spatial)
  * If necessary, add new interpolation points using the monitor function and θ_{r}

UNTIL the set of interpolation points remains fixed

* Accept time step and new solution

Meshfree integrator

As an example, consider a linear differential equation

$$\partial_t u(t,\xi) = Au(t,\xi)$$

Approximate $Au(t,\xi)$ by

$$As(t,\xi) = A\sum_{\eta\in H}\lambda_\eta(t)\Phi\big(\xi-\eta\big) = \sum_{\eta\in H}\lambda_\eta(t)A\Phi\big(\xi-\eta\big).$$

This gives

$$\partial_t s(t,\cdot)|_H = B_A B^{-1} s(t,\cdot)|_H \qquad \text{linear ODE}$$

$$B_A = \Big(A\Phi\big(\eta_i-\eta_j\big)\Big)_{\{\eta_i,\eta_j\}\in H} \qquad B = \Big(\Phi\big(\eta_i-\eta_j\big)\Big)_{\{\eta_i,\eta_j\}\in H}$$

Caliari, A.O., Rainer (2010)

Example: Molenkamp–Crowley

Consider the Molenkamp–Crowley equation

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

with

$$a(x,y) = 2\pi y, \quad b(x,y) = -2\pi x$$

The initial pulse

$$u_0(x,y) = \exp\bigl(-10(x-0.2)^2 - 10(y-0.2)^2\bigr)$$

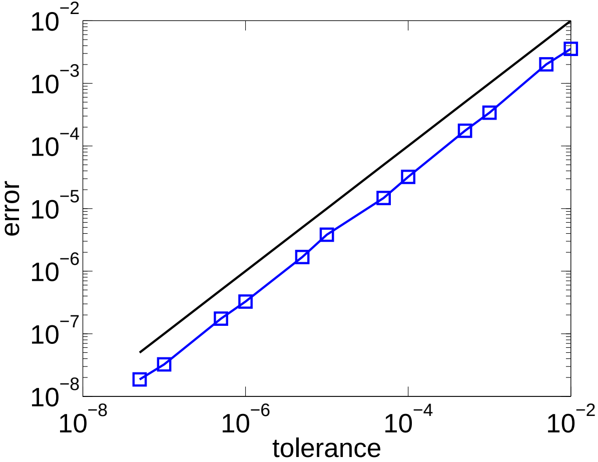
rotates in time $t = 1$ once around the origin.

Two numerical experiments

- achieved accuracy (in terms of prescribed tolerance)
- long term computation

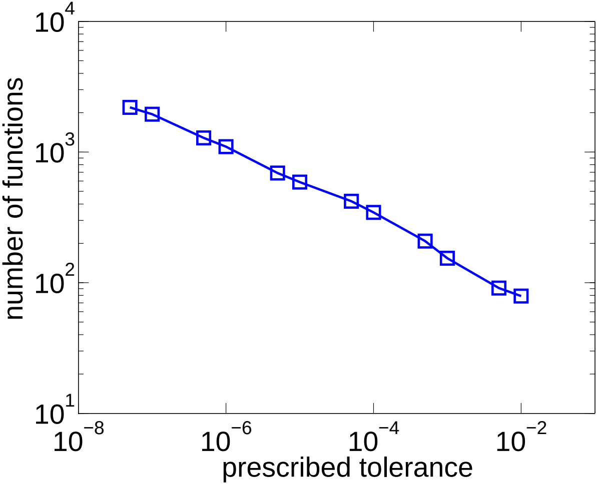
Only spatial error (exponential integrator is exact in time).

Global error at $t = 1$

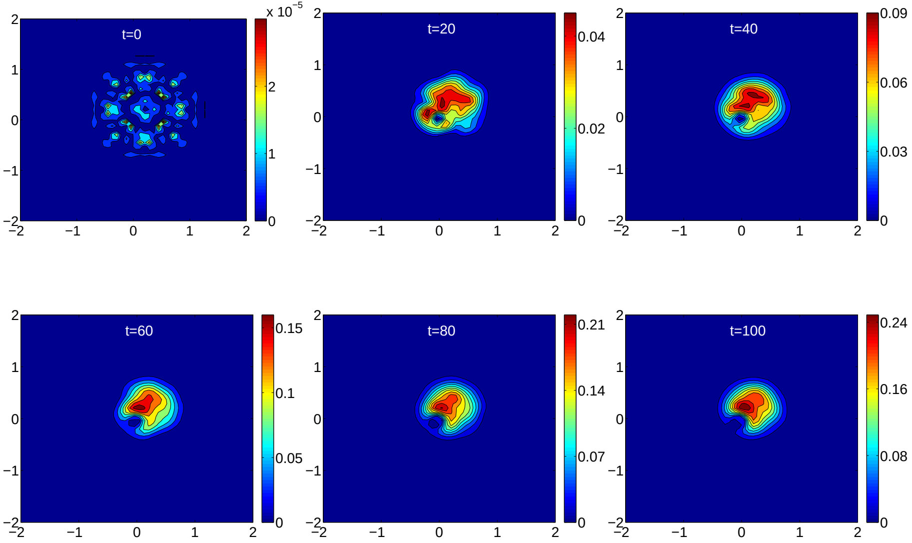


Achieved accuracy at $t = 1$ as function of prescribed tolerance

Required number of radial basis functions



Long term integration (100 turns)



Nonlinear Schrödinger equations, soliton dynamics

Nonlinear Schrödinger equation in the semi-classical regime

$$\mathrm{i}\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + V(x,y)\psi - |\psi|^{2p}\psi, \qquad (x,y)\in\mathbb{R}^2$$

with $\varepsilon = 0.01$, $p = 0.2$ and the harmonic potential

$$V(x,y) = ax^2 + by^2, \quad a = 1.5,\ b = 1$$

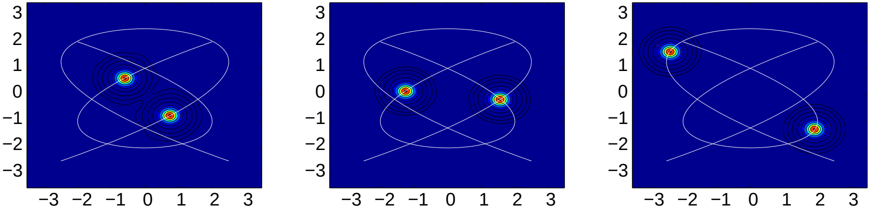
(relevant in the theory of Bose–Einstein condensates);
solitary waves move on Lissajous curves.

Space discretization: radial basis functions

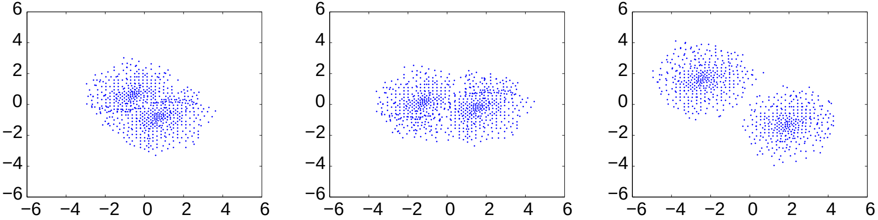
Time discretization: splitting method

Caliari, Squassina (2010); Caliari, A.O., Rainer (2011)

Soliton dynamics, numerical example



$t = 1.25$ $\qquad$ $t = 1.5$ $\qquad$ $t = 4$



Linearised exponential integrators

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

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

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

- Apply a standard explicit exponential method

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

The exponential Rosenbrock–Euler method

Applying the exponential Euler method to

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

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

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

The method has order two.

Linearised exponential multistep methods

Example (Tokman 2006)

$$u_{n+1} = u_n + h\,\varphi_1(hJ_n)F(u_n) - \frac{2h}{3}\varphi_2(hJ_n)\big(g_n(u_n) - g_n(u_{n-1})\big)$$

perturbed exponential Rosenbrock–Euler step, order three

Variant (Hochbruck, O. 2010)

$$u_{n+1} = u_n + h\,\varphi_1(hJ_n)F(u_n) - 2h\,\varphi_3(hJ_n)\big(g_n(u_n) - g_n(u_{n-1})\big)$$

For $J_n = 0$, both methods coincide; the latter, however, has better uniform convergence properties.

Apply exponential Adams methods to the locally linearised equation $\longrightarrow$ *linearised exponential multistep methods*

Exponential Rosenbrock-type methods

For the locally linearized problem

$$u'(t) = F\big(u(t)\big) = J_n u(t) + g_n\big(u(t)\big), \quad u(t_n) = u_n$$

we consider

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

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

with small

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

(Hochbruck, Schweitzer, O. 2006, 2009)

Embedded methods of order 3 and 4

erow32: Third-order method with second-order error estimate

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

erow43: Fourth-order method with third-order error estimate

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

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

Approach based on interpolation methods.

- Approximate $\exp(hJ)v$ by an interpolation polynomial; involves only matrix-vector multiplications; short recurrences. Estimate on spectrum required.
- Sensitivity of the interpolation polynomial strongly depends on the interpolation nodes.
- Real (and complex) Leja points are an attractive choice (Leja 1957, Reichel 1990)
  - distributed in a similar way as Chebyshev points;
  - defined recursively - fits well to Newton interpolation;
  - superlinear convergence.

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

Conclusions

- Fully adaptive integrator
- Applicable to various evolution equations
- Small essential support essential
- Particularly efficient in high dimensions
- Combines well with splitting methods and exponential integrators
- Open problem: boundary conditions