Partitioned Runge–Kutta methods in space and time

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Outline

- Runge–Kutta methods
- partitioned
- in time
- and space

Runge–Kutta methods

For the ODE $\dot{x} = f(x),\ x \in \mathbb{R}^n$, an s-stage RK method $x_0 \mapsto x_1$ is defined by

$$X_i = x_0 + \Delta t \sum_{i=1}^{s} a_{ij} f(X_j)$$

$$x_1 = x_0 + \Delta t \sum_{i=1}^{s} b_j f(X_j)$$

Covariance

An integrator φ is h-covariant if the diagram commutes.

$$\begin{array}{ccc}
\dot{x} = f(x) & \overset{x \mapsto h(x)}{\longrightarrow} & \dot{x} = (Dh.f) \circ h^{-1} \\
\varphi \downarrow & & \varphi \downarrow \\
x \mapsto \varphi_f(x) & \overset{x \mapsto h(x)}{\longrightarrow} & \begin{array}{l} x \mapsto \varphi_{(Dh.f)\circ h^{-1}}(x) \\ \quad = h \circ \varphi_f \circ h^{-1}(x) \end{array}
\end{array}$$

RK methods are linearly (and affine) covariant.

Properties of RK

- Any linear symmetries are preserved.
- If $a_{ij} + a_{s+1-i,s+1-j} = b_j$, the method is symmetric ($\varphi_{\Delta t}\varphi_{-\Delta t} = 1$) and any linear reversing symmetries are preserved. The method is nondissipative for all Δt.
- If $b_i a_{ij} + b_j a_{ji} + b_i b_j = 0$, any constant symplectic structure, any constant Poisson structure, and any quadratic first integrals are preserved. The method is nondissipative for all Δt.
  - Main example: Gauss RK = collocation at Gauss quadrature nodes.
    - A-stable (stable on $\dot{x} = \lambda x \,\forall\, \Delta t,\ Re(\lambda) \leq 0$)
    - Maximal order $2s$.
    - Frequency response ($\dot{x} = i\omega x$, $x \mapsto e^{i\phi(\Delta t\omega)}x$) is monotonic ($\phi' > 0$).

Approaches to geometric integration

- Enforce the desired property
- Assume & exploit the property during design
- Find methods which naturally preserve the desired property

Partitioned RK methods

For $x = (q, p)$, $\dot{q} = f(q, p)$, $\dot{p} = g(q, p)$, a PRK method is

$$Q_i = q_0 + \Delta t \sum_{i=1}^{s} a_{ij} f(Q_j, P_j)$$

$$P_i = p_0 + \Delta t \sum_{i=1}^{s} \tilde{a}_{ij} g(Q_j, P_j)$$

$$q_1 = q_0 + \Delta t \sum_{j=1}^{s} b_j f(Q_j, P_j)$$

$$p_1 = p_0 + \Delta t \sum_{j=1}^{s} \tilde{b}_j g(Q_j, P_j)$$

Putative application

Canonical Hamiltonian system:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

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$$b_i = \tilde{b}_i, \qquad b_i \tilde{a}_{ij} + \tilde{b}_j a_{ji} - b_i \tilde{b}_j = 0$$

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- 2003: Grimm & Scherer construct all high-order symplectic PRK methods.
- 2006: Jay modifies Gauss RK so that order $2s$ is recovered for constrained systems.

Lobatto IIIA–IIIB PRK methods

$(s=2):$ IIIA:
$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array},$$
IIIB:
$$\begin{array}{c|cc} 0 & \frac{1}{2} & 0 \\ 1 & \frac{1}{2} & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

$(s=3):$ IIIA:
$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array},$$
IIIB:
$$\begin{array}{c|ccc} 0 & \frac{1}{6} & -\frac{1}{6} & 0 \\ \frac{1}{2} & \frac{1}{6} & \frac{1}{3} & 0 \\ 1 & \frac{1}{6} & \frac{5}{6} & 0 \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

Generalized leapfrog

2-stage, order 2 Lobatto IIIA-B method can be written as

$$Q = q_0 + \frac{\Delta t}{2} f(Q, p_0)$$

$$p_1 = p_0 + \frac{\Delta t}{2} (g(Q, p_0) + g(Q, p_1))$$

$$q_1 = Q + \frac{\Delta t}{2} f(Q, p_1)$$

- Less implicit than midpoint rule
- Extends leapfrog to nonseparable systems
- Widely used in constrained and adaptive geometric integration

A natural derivation of PRK

Lagrangian system $\mathcal{L} = \int_{t_0}^{t_1} L(q(t), \dot{q}(t))\, dt$.

Let (b_j, c_j) be a set of quadrature weights and nodes.

Let

$$\mathcal{L}_d = \Delta t \sum_{j=1}^{s} b_j L(u(c_j \Delta t), \dot{u}(c_j \Delta t)).$$

Marsden & West:

- Extrema of $\mathcal{L}_d$ over polynomials u with $u(0) = q_0$, $u(1) = q_1$ yield symplectic PRK methods.
- Order = quadrature order.
- Gauss quadrature yields Gauss RK.
- Lobatto quadrature yields Lobatto IIIA–IIIB.

Stability in time integration

Any study of stability requires a test problem, e.g. $\dot{x} = Ax$. RK method gives $x_1 = R(\Delta t A)x_0$, where

$$R : \mathbb{C} \mapsto \mathbb{C}, \quad R(z) = 1 + zb(I - zA)^{-1}\mathbf{1}.$$

Usually assume that A is diagonalizable; then

$$\{R(\Delta t\lambda) \colon \lambda \in \sigma(A)\}$$

completely determines the behaviour of the method, and in particular its stability.

Nondiagonalizable case

Theorem An RK method with stability function $R(z)$ applied to a linear system with matrix given by a Jordan block with eigenvalue λ yields a linear map whose matrix is upper triangular with constant diagonals such that the kth diagonal is equal to

$$\frac{(\Delta t)^k}{k!} R^{(k)}(\Delta t \lambda).$$

$$\begin{pmatrix} \lambda & 1 & 0 & \dots \\ 0 & \lambda & 1 & 0 \\ \vdots & & & \end{pmatrix} \longrightarrow \begin{pmatrix} R(\Delta t\lambda) & \Delta t R'(\Delta t\lambda) & \frac{1}{2}(\Delta t)^2 R''(\Delta t\lambda) & \dots \\ 0 & R(\Delta t\lambda) & \Delta t R'(\Delta t\lambda) & \\ \vdots & & & \end{pmatrix}$$

Stability of PRK

What is the normal form of partitioned linear systems

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

under partitioned linear maps

$$q \mapsto X_1 q, \quad p \mapsto X_2 p \quad ?$$

Partitioned ODEs can't be diagonalized

New system is

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} X_1^{-1} A X_1 & X_1^{-1} B X_2 \\ X_2^{-1} C X_1 & X_2^{-1} D X_2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

Partitioned ODEs can't be diagonalized

New system is

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} X_1^{-1}AX_1 & X_1^{-1}BX_2 \\ X_2^{-1}CX_1 & X_2^{-1}DX_2 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}$$

. . . or block diagonalized.

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. . . or block diagonalized.

. . . even in the Hamiltonian case

$$B = B^T, \quad C = C^T, \quad D = -A^T, \quad X_j \text{ arbitrary}.$$

A possible normal form

Suppose B is invertible. First let $X_1 = B$, $X_2 = I$ to get

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} B^{-1}AB & I \\ CB & -A^T \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}.$$

CB is similar to the symmetric matrix $B^{1/2}CB^{1/2}$, hence diagonalizable. Let $X_2 = X_1$, $X_1^{-1}CBX_1 = \Lambda$, giving

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} X_1^{-1}B^{-1}ABX_1 & I \\ \Lambda & -X_1^{-1}A^TX_1 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}.$$

The separable case $A = 0$ gives 2D subsystems $\ddot{q}_i = \lambda_i q_i$. Harmonic oscillators when $\lambda_i < 0$.

2D linear symplectic maps

Consider $x \mapsto Rx$, $x \in \mathbb{R}^2$.

Eigenvalues are $\frac{\operatorname{tr} R}{2} \pm \sqrt{(\frac{\operatorname{tr} R}{2})^2 - \det R}$.

For a symplectic map, $\det R = 1$; stability if $|\operatorname{tr} R| \leq 2$.

For the exact solution of the harmonic oscillator,

$$R = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}$$

$$\operatorname{tr} R = 2 \cos t$$

Nonseparability: 2D case

A normal form is

$$\dot{x} = \begin{pmatrix} \mu & \omega \\ -\omega & -\mu \end{pmatrix} x, \quad \text{evs } \pm i\sqrt{\omega^2 - \mu^2}.$$

Stable when $|\mu| \le |\omega|$.
Generalized leapfrog gives

$$x \mapsto \frac{1}{4-\mu^2} \begin{pmatrix} 4+\mu^2-2\omega^2+4\mu & 4\omega \\ \omega(-4-\mu^2+\omega^2) & 4+\mu^2-2\omega^2-4\mu \end{pmatrix} x$$

with trace ≤ 2 when

$$|\omega| \le 2 \text{ and } |\mu| \le |\omega|.$$

- nonseparability (μ) does not affect stability

Nonseparability: 2D case

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$$\dot{x} = \begin{pmatrix} \mu & \omega \\ -\omega & -\mu \end{pmatrix} x, \quad \text{evs } \pm i\sqrt{\omega^2 - \mu^2}.$$

Stable when $|\mu| \leq |\omega|$.
4th order Lobatto is stable when

$$\omega \leq \mu, \quad \omega \leq \sqrt{24}, \text{ and } \frac{\omega^2}{12 + \mu^2} \notin \left(\frac{2}{3}, 1\right).$$

- nonseparability (μ) does affect the stability

Multi-Hamiltonian systems

The PDE

$$\mathbf{K}z_t + \mathbf{L}z_x = \nabla S(z), \quad z \in \mathbb{R}^n, \quad \mathbf{K}^T = -\mathbf{K}, \quad \mathbf{L}^T = -\mathbf{L}$$

has the differential conservation law

$$\omega_t + \kappa_x = 0$$

$$\omega = dz \wedge \mathbf{K}dz, \quad \kappa = dz \wedge \mathbf{L}dz$$

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(Proof:

$$\omega_t + \kappa_x = 2(dz \wedge \mathbf{K}dz_t + dz \wedge \mathbf{L}dz_x) = 2dz \wedge S''(z)dz = 0$$)

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Discrete analogue: a multisymplectic integrator, e.g.

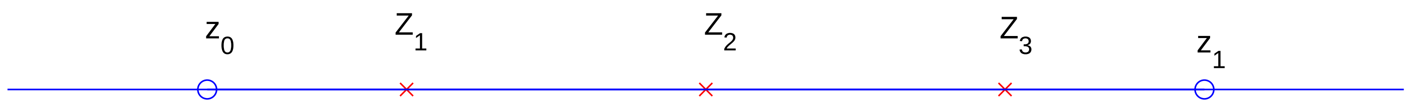
$$\Delta_t\omega + \Delta_x\kappa = 0.$$

Spatial discretization by RK

Sebastian Reich, Multisymplectic Runge-Kutta collocation methods for Hamiltonian wave equations, J Comput Phys 2000.

- Any symplectic integrator applied in space and in time yields a scheme with a discrete multisymplectic conservation law.
- Any symmetric integrator applied in space and in time yields a scheme with a discrete multisymplectic conservation law.
- Moore & Reich define a multisymplectic integrator as one coming from a 1-step symplectic integrator in space and in time.

Spatial discretization by RK



Node grid points x_i, values z_i
Stage grid points $x_i + c_j \Delta x$, values Z_j

Spatial discretization by RK

$$Z_j = z_0 + \Delta x \sum_{l=1}^{r} a_{jl} \partial_x Z_l, \quad j = 1, \ldots, r,$$

$$z_1 = z_0 + \Delta x \sum_{l=1}^{r} b_l \partial_x Z_l$$

$$\mathbf{K} Z_{l,t} + \mathbf{L} \partial_x Z_l = \nabla S(Z_l), \quad l = 1, \ldots, r.$$

A set of DAEs.

(a_{jl}, b_l coefficients of a symplectic method.)

Multisymplecticity of spatial RK

Any solutions (Z_j, z_i) formally satisfy

$$\sum_{j=1}^{r} b_j(\omega_j)_t + \kappa_1 - \kappa_0 = 0$$

where

$$\omega_j = dZ_j \wedge \mathbf{K} dZ_j, \quad \kappa_i = dz_i \wedge \mathbf{L} dz_i$$

which is an approximation of

$$\int_{x_0}^{x_1} \omega_t \, dx + \kappa_1 - \kappa_0 = 0$$

which is the integral of

$$\omega_t + \kappa_x = 0.$$

Spatial discretization by RK

If the operator $(1b^{\mathrm{T}} + A\Delta)$ is nonsingular then we formally invert it to write

$$\mathbf{K}Z_t + (\Delta x)^{-1}(\mathbf{1}b^{\mathrm{T}} + A\Delta)^{-1}\Delta\mathbf{L}Z = \nabla S(Z).$$

- Yields implicit ODEs
- Geometry w.r.t $(\mathbf{K}, \mathbf{L}, S)$ is preserved
- RK = continuous Galerkin w/ quadrature (Lesaint and Raviart, Math. Comp. 1979)
- Operator may be singular: for periodic boundary conditions, nonsingularity requires N and r both odd.

Dispersion analysis: continuous

Continuous dispersion:

$$\mathbf{K}z_t + \mathbf{L}z_x = Sz$$

$$z = \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}kx}\tilde{z}$$

$$(i\omega\mathbf{K} + \mathrm{i}k\mathbf{L} - S)\tilde{z} = 0$$

$$\det(\mathrm{i}\omega\mathbf{K} + \mathrm{i}k\mathbf{L} - S) = 0$$

Dispersion analysis: discrete

Discrete dispersion: $(z_i, Z_j) = \mathrm{e}^{\mathrm{i}\omega t}\mathrm{e}^{\mathrm{i}Kx_i}(\tilde{z}_i, \tilde{Z}_j)$

Ascher & M 2004, Frank Moore Reich 2006, M 2007:
Gauss RK preserves the dispersion relation unconditionally up to a monotonic relabelling of frequencies.

$$\det(\mathrm{i}\omega\mathbf{K} + \mathrm{i}K\mathbf{L} - S) = 0$$

$$\mathrm{e}^{\mathrm{i}K\Delta x} = R(\mathrm{i}k\Delta x) = \mathrm{e}^{\mathrm{i}\phi(k\Delta x)}$$

$$\phi : (-\infty, \infty) \to (-s\pi, s\pi),\ \phi' > 0$$

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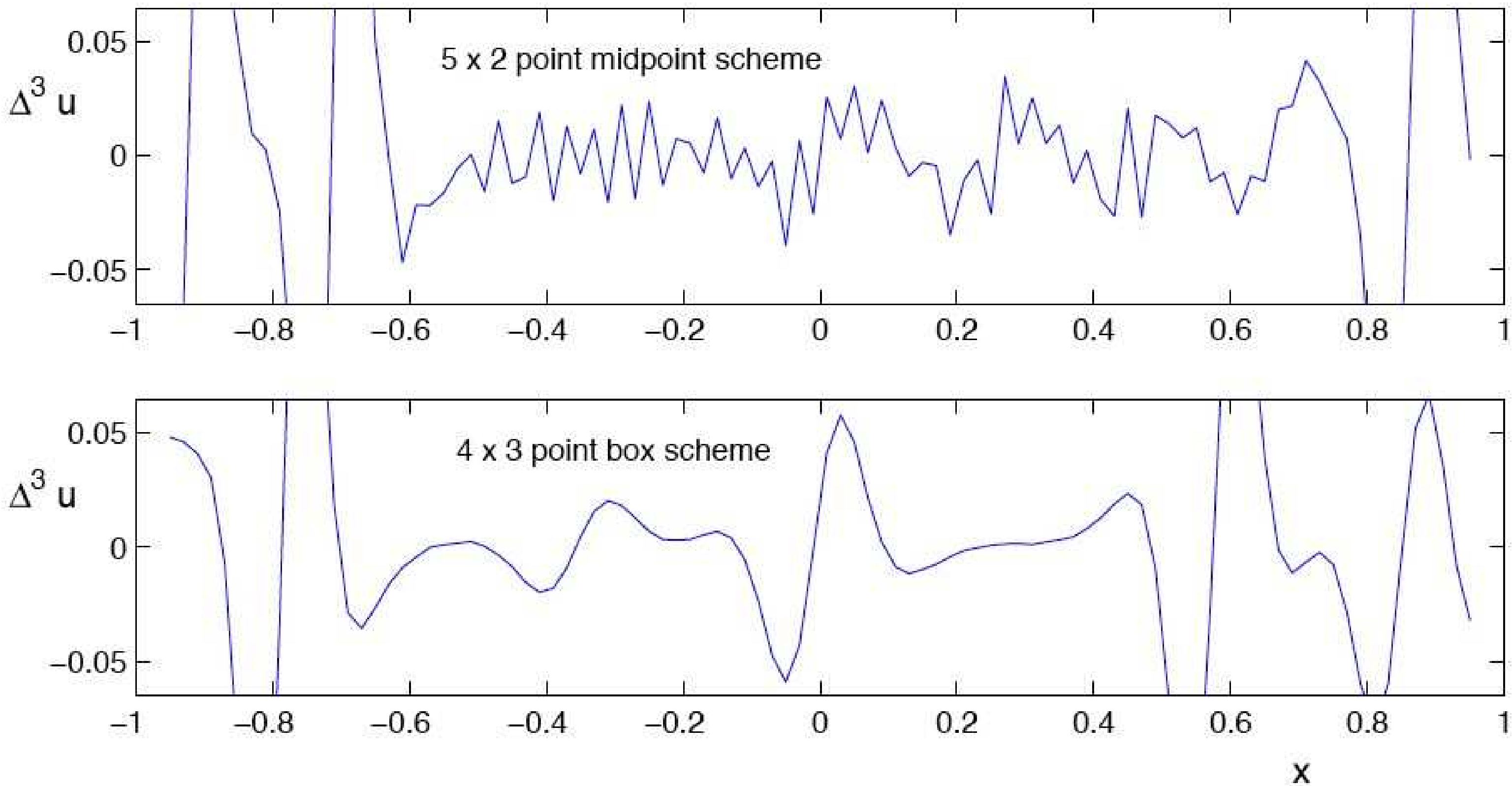
$$\phi : (-\infty, \infty) \to (-s\pi, s\pi),\ \phi' > 0$$

- Number of branches of dispersion relation preserved
- no parasitic waves for any Δx
- sign of group velocity preserved

Example: KdV equation



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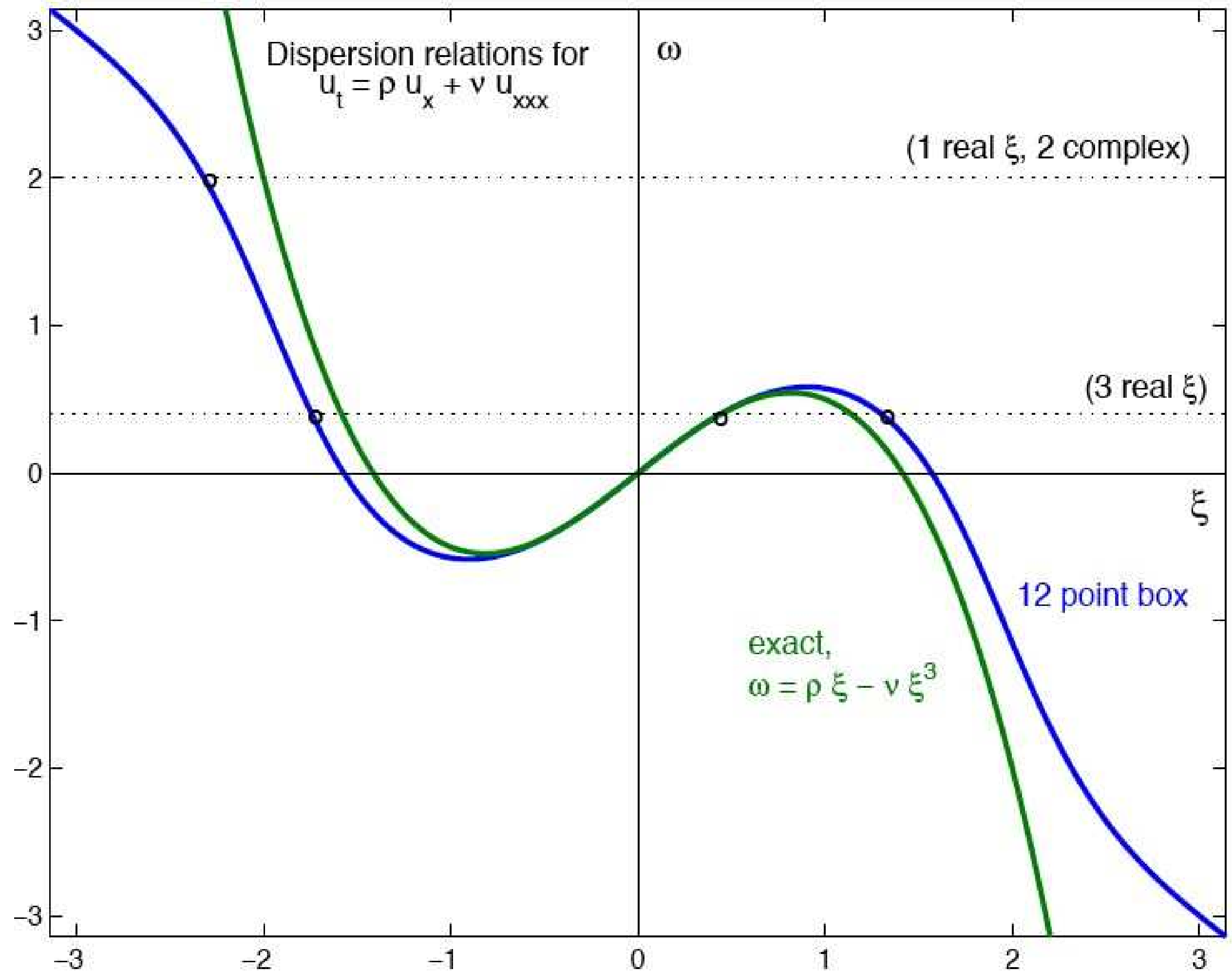


RK frequency mapping

Recall

$$e^{iK\Delta x} = R(ik\Delta x) = e^{i\phi(k\Delta x)}$$

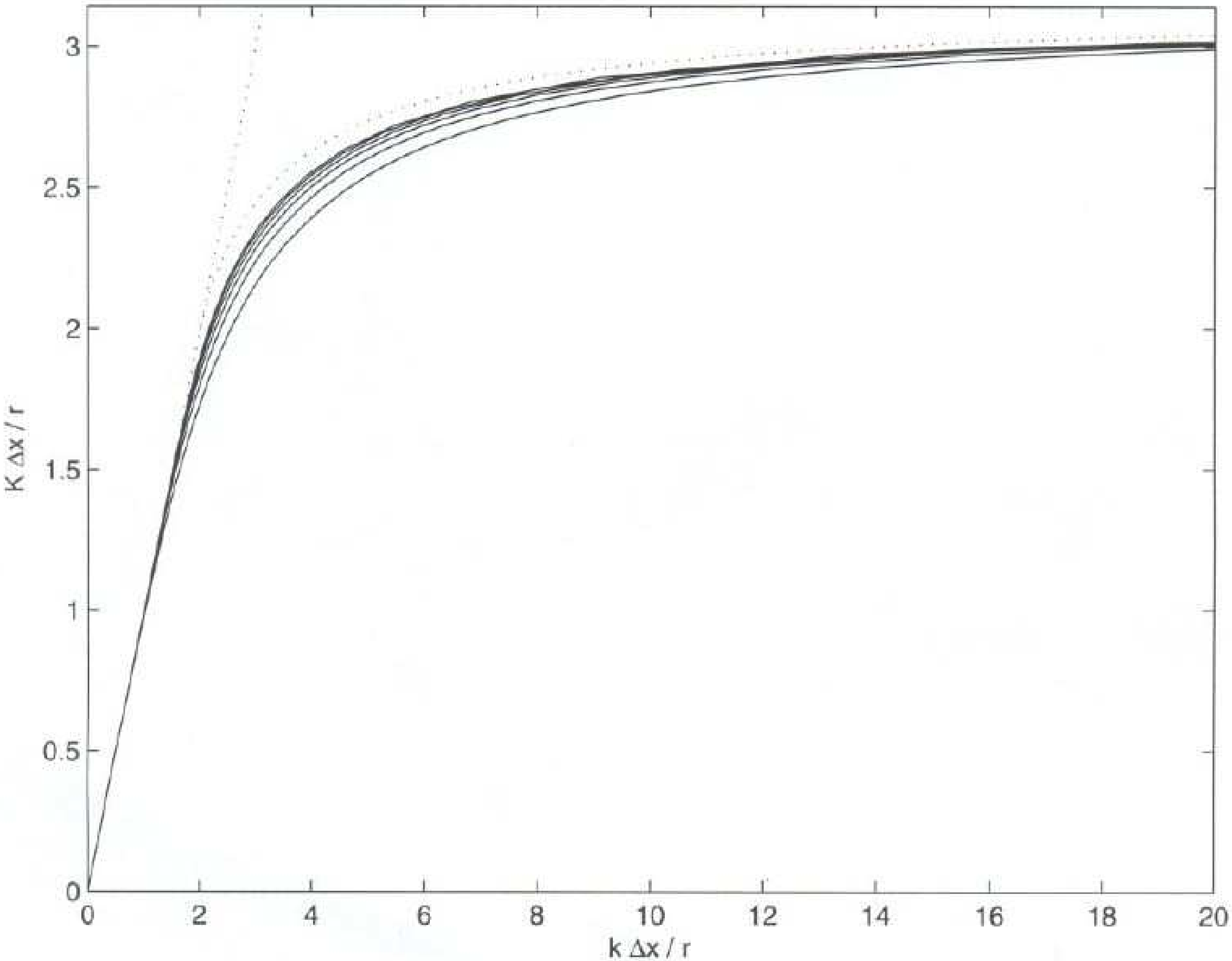
$$\arg R(ik\Delta x) \approx \begin{cases} k\Delta x & k \to 0 \\ s\pi & k \to \infty \end{cases}$$

so

$$\arg R(iks\Delta x)/s \approx \begin{cases} k\Delta x & k \to 0 \\ \pi & k \to \infty \end{cases}$$

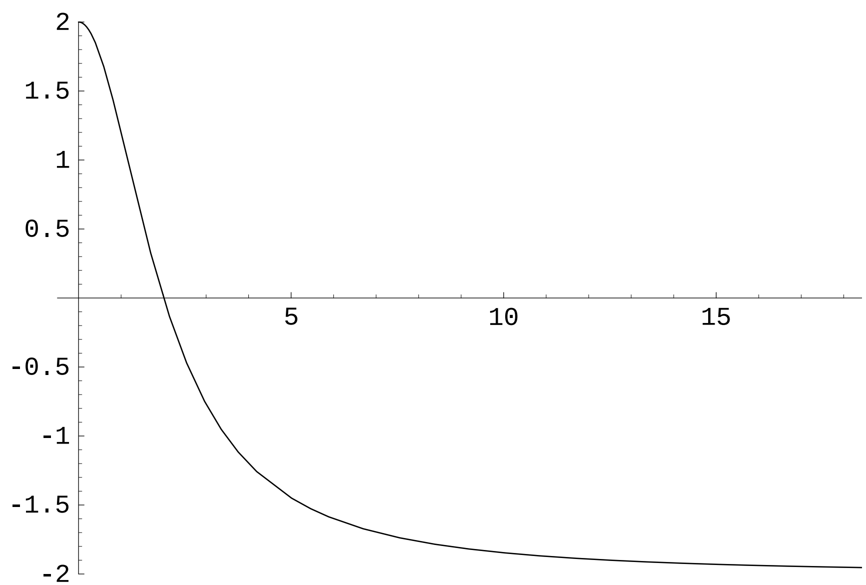
But what happens for fixed k as $s \to \infty$?

RK frequency mapping



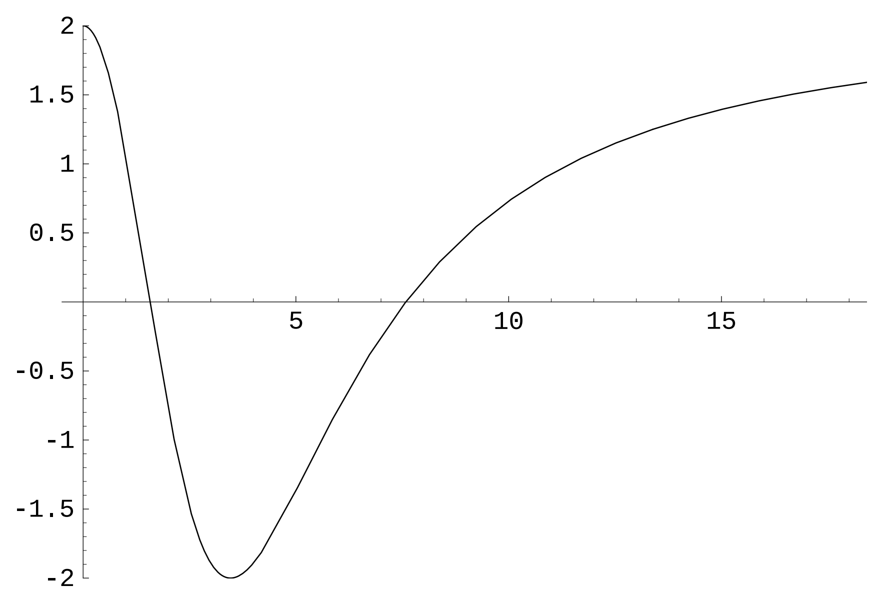
Symplectic RK on harmonic oscillator

$s = 1$ (midpoint rule)



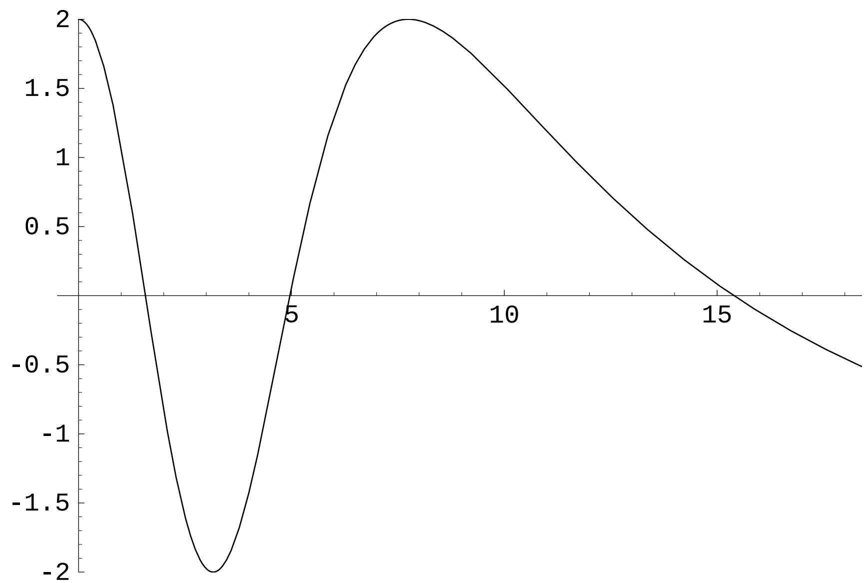
Symplectic RK on harmonic oscillator

$s = 2$ stages, 4th order



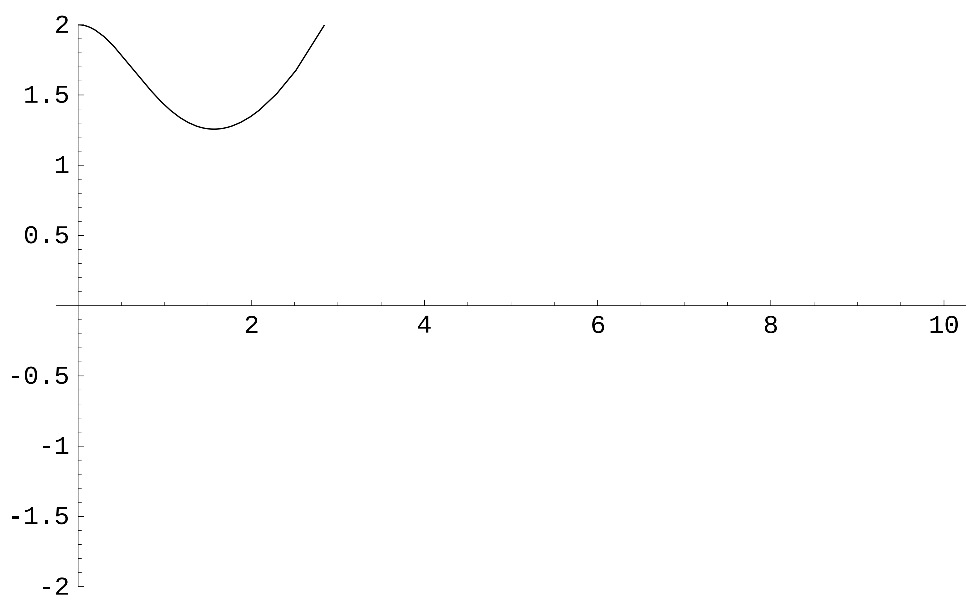
Symplectic RK on harmonic oscillator

$s = 3$ stages, 6th order



Symplectic RK on harmonic oscillator

$s = 2$ stages, not Gauss: unstable



Large s limit

We need to study $\log R(sz)/s$ for fixed z and $s \to \infty$, where $R(z)$ is the diagonal Padé approximation to e^z (Hermite 1873).

Saff and Varga 1975: Let $w(z) = \frac{z\mathrm{e}^{\sqrt{1+z^2/4}}}{2(1+\sqrt{1+z^2/4})}$.

Zeros and poles cluster along $C = \{z : |w(z)| = 1, \quad |z| \leq 2\}$.

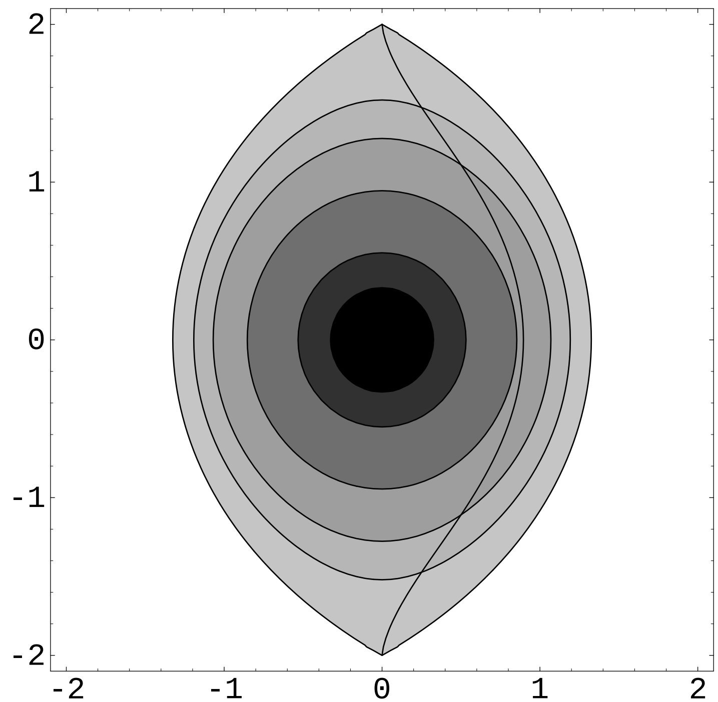
Wong and Zhang 1997:

$$\lim_{s\to\infty} \frac{\log R_s(sz)}{s} = \begin{cases} z & \text{inside } C \\ z - 2\log w(z) & \text{outside } C \\ \sim \frac{2}{z} - \frac{2}{3z^3} + \frac{4}{5z^5} - \dots & z \to \infty \end{cases}$$

which is differentiable (but not twice differentiable) at $z = 2\mathrm{i}$:

$$\lim_{s\to\infty} \log R_s(sz)/s = z + \mathcal{O}((z-2\mathrm{i})^{3/2}), \qquad z \to 2\mathrm{i}.$$

The eye ($R_s(sz) \to e^{sz}$, $s \to \infty$)



Large s limit

Conclusion:

The dispersion relation is correct for frequencies up to $2s$, while the grid supports frequencies up to πs.

Consistent with the fact that the largest grid spacing, near the cell midpoints, is asymptotically $\frac{\pi}{2s}$, a spacing which, at 2 grid points per period, can support frequencies up to $2s$.

Eigenfunctions

- On uniform grids, the discrete eigenfunctions $\mathrm{e}^{\mathrm{i}kx_j}$ coincide with the continuous eigenfunctions $\mathrm{e}^{\mathrm{i}kx}$ evaluated on the grid.
- This is no longer true on nonuniform grids
- The dispersion relation no longer carries all the information in the linear case
- For Gauss RK, the phases of the high frequency eigenfunctions are nearly correct, but the amplitudes are not.

Disadvantages of RK

- Speed $\to \infty$ as $K\Delta x \to s\pi$. ODEs extremely stiff. There may be a $\Delta t < CN^{-2}$ nonlinear stability restriction, even when integrating by Gauss RK.
- ODEs are implicit.

Boundary conditions. . .

. . . are a problem.

For example, with periodic boundary conditions, the ODEs are only well-defined if N and s are both odd.

$$\frac{1}{4}[1\ 2\ 1]\partial_t u_i = \frac{1}{(\Delta x)^2}[1\ \ -2\ 1]u_i - V'(u_i)$$

Mass matrix annihilates sawtooth $(-1)^j$.

Dirichlet and Neumann boundary conditions can lead to counting problems.

PRK

Partitioned Runge–Kutta offers a way out of some of these problems.
Good points:

- Can be multisymplectic
- Lobatto IIIA-IIIB can give explicit ODEs.
- L IIIA-IIIB is stable and less stiff than Gauss RK ($\Delta t < C\Delta x$)
- It yields local, nonsingular methods for various boundary conditions

Leapfrog

The simplest symplectic integrator for $u_{tt} = -V'(u)$ is leapfrog:

$$\frac{1}{(\Delta t)^2}\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} u = -V'(u)$$

which for $u_{tt} - u_{xx} = -V'(u)$ gives the explicit multisymplectic integrator

$$\frac{1}{(\Delta t)^2}\begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix} u - \frac{1}{(\Delta x)^2}\begin{bmatrix} 1 & -2 & 1 \end{bmatrix} u = -V'(u),$$

How does this generalize?

Partitioned Runge–Kutta methods

Theorem: A multi-Hamiltonian PDE discretised by PRK methods $(a_{jk}^{(\beta)}, b^{(\beta)})$ in space and $(A_{jk}^{(\beta)}, B^{(\beta)})$ in time has a discrete multisymplectic conservation law

$$\Delta x \sum_j b_j(\omega_{i,j}^{n+1} - \omega_{i,j}^{n}) + \Delta t \sum_m B_m(\kappa_{i+1}^{n,m} - \kappa_i^{n,m}) = 0,$$

where

$$\omega_{i,j}^n = \frac{1}{2}\sum_{\beta,\gamma} K_{\beta\gamma} \mathrm{d}Z_{i,j}^{\gamma,n} \wedge \mathrm{d}Z_{i,j}^{\beta,n}, \quad \kappa_i^{n,m} = \frac{1}{2}\sum_{\beta,\kappa} L_{\beta\gamma} \mathrm{d}Z_i^{\gamma,n,m} \wedge \mathrm{d}Z_i^{\beta,n,m}$$

when

$$b_j^{(\gamma)} = b_j, \; -a_{kj}^{(\gamma)} b_k^{(\beta)} - b_j^{(\gamma)} a_{jk}^{(\beta)} + b_j^{(\gamma)} b_k^{(\beta)} = 0$$

for all j, k, β, γ such that $L_{\beta\gamma} \neq 0$ and

$$B_m^{(\gamma)} = B_m, \; -A_{nm}^{(\gamma)} B_n^{(\beta)} - B_m^{(\gamma)} A_{mn}^{(\beta)} + B_m^{(\gamma)} B_n^{(\beta)} = 0$$

for all m, n, β, γ such that $K_{\beta\gamma} \neq 0$.

Explicit spatial discretization

Theorem: Let

$$K = \begin{bmatrix} & -I_{\frac{1}{2}(d_1+d_2)} & \\ I_{\frac{1}{2}(d_1+d_2)} & & \\ & & 0_{d_1} \end{bmatrix}, \qquad L = \begin{bmatrix} & & I_{d_1} \\ & 0_{d_2} & \\ -I_{d_1} & & \end{bmatrix}$$

and

$$S(z) = S(p,q,v) = \frac{1}{2}p^t\beta p + V(q) + \frac{1}{2}v^T\alpha v, \quad |\alpha| \neq 0, \quad |\beta| \neq 0$$

then applying an s-stage Lobatto IIIA–IIIB PRK discretisation in space to the PDE leads to a set of explicit local ODEs in time in the stage variables associated with q.

Example: Nonlinear wave equation

$$u_{tt} = u_{xx} - V'(u),$$

$$z = \begin{bmatrix} u \\ v \\ w \end{bmatrix}, \quad K = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$$

$$S(z) = V(u) + \frac{1}{2}v^2 - \frac{1}{2}w^2.$$

$s = 3$ gives the explicit ODEs

$$\partial_t^2 U_{i,1} = \frac{1}{(\Delta x)^2}(-U_{i-1,1} + 8U_{i-1,2} - 14U_{i,1} + 8U_{i,2} - U_{i+1,1}) - V'(U$$

$$\partial_t^2 U_{i,2} = \frac{1}{(\Delta x)^2}(4U_{i,1} - 8U_{i,2} + 4U_{i+1,1}) - V'(U_{i,2}),$$

NLS equation

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0,\ \psi = q + ip,\ \psi_x = v + iw$$

$$z = \begin{bmatrix} p \\ q \\ v \\ w \end{bmatrix}, \quad K = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

$$S = -\frac{1}{2}(p^2 + q^2)^2 - \frac{1}{2}(v^2 + w^2).$$

NLS equation

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$$S = -\frac{1}{2}(p^2 + q^2)^2 - \frac{1}{2}(v^2 + w^2).$$

$s = 2$ gives

$$i\partial_t\psi_i = -\frac{1}{(\Delta x)^2}(\psi_{i-1} - 2\psi_i + \psi_{i+1}) - 2|\psi_i|^2\psi_i$$

NLS equation

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0,\ \psi = q + ip,\ \psi_x = v + iw$$

$$z = \begin{bmatrix} p \\ q \\ v \\ w \end{bmatrix}, \quad K = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

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$s = 3$ gives

$$i\partial_t\psi_{i,1} = -\frac{1}{(\Delta x)^2}(-\psi_{i-1,1} + 8\psi_{i-1,2} - 14\psi_{i,1} + 8\psi_{i,2} - \psi_{i+1,1}) - 2|$$

$$i\partial_t\psi_{i,2} = -\frac{1}{(\Delta x)^2}(4\psi_{i,1} - 8\psi_{i,2} + 4\psi_{i+1,1}) - 2|\psi_{i,2}|^2\psi_{i,2}$$

Korteweg-de Vries (KdV) equation

$$u_t = V'(u)_x + \nu u_{xxx}$$

$$z = \begin{bmatrix} u \\ \phi \\ v \\ w \end{bmatrix}, \quad K = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$$

and with $S(z) = -\frac{1}{2}uw - V(u) - \frac{1}{2\nu}v^2$.
K, L have the required structure, but S does not.

Taking $s = 2$ and eliminating ϕ, v, and w gives the implicit ODEs

$$\frac{1}{2}[1\ 1]\partial_t u_i = \frac{1}{\Delta x}[-1\ 1]V'(u_i) + \nu(\frac{1}{\Delta x}[-1\ 1])^3 u_{i-1}.$$

Boundary conditions

The ODEs remain well-defined under periodic, Dirichlet and Neumann boundary conditions.

Example: NLS, $s = 3$, BC $\psi_x(0) = 0$ leads to

$$i\partial_t \psi_{1,1} = -\frac{1}{(\Delta x)^2}(-14\psi_{1,1} + 16\psi_{1,2} - 2\psi_{2,1}) - 2|\psi_{1,1}|^2\psi_{1,1},$$

while $\psi_{1,2}$ does not require a boundary condition.

Dispersion under PRK

We cannot expect such a general result as for RK, because of nonseparability. In the case for which PRK can lead to explicit ODEs, the linearized PDE can be put in the form

$$q_{xx} = f(q, q_t)$$

or, with $q = \mathrm{e}^{\mathrm{i}\omega t}\tilde{q}$,

$$\tilde{q}_{xx} = \tilde{f}(\tilde{q}),$$

a set of harmonic oscillators.

Theorem For these PDEs, the PRK dispersion relation is conjugate to the continuous dispersion relation, according to

$$\mathrm{tr}\, R(k\Delta x) = 2\cos(K\Delta x) \qquad (*)$$

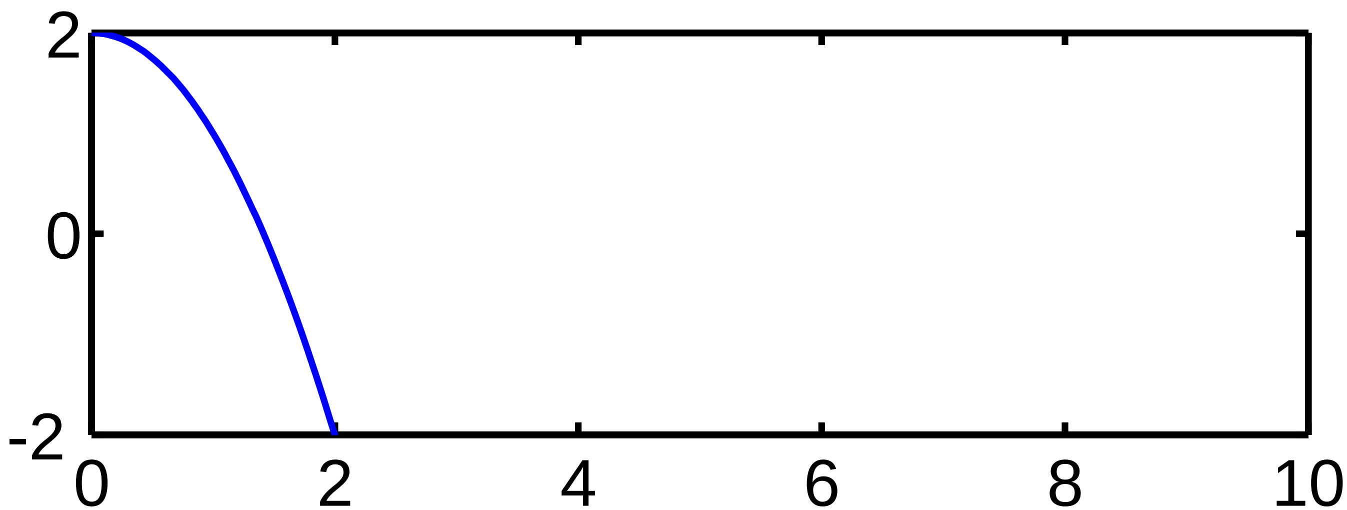
Dispersion under PRK

$$\operatorname{tr} R(k\Delta x) = 2\cos(K\Delta x) \qquad (*)$$

- The conjugacy is monotonic but not necessarily continuous or onto $k \in (-\infty, \infty)$.
- A PRK method with s dependent variables per cell is stable if to each $K\Delta x \in (-\pi, \pi)$ there are exactly s solutions $k\Delta x$ to $(*)$.
- Let $k^* = \max\{k : |\operatorname{tr} R(k)| = 2\}$. Only frequencies up to $k^*/\Delta x$ are captured. Dispersion relation qualitatively correct only for sufficiently small Δx.
- k^* determines the speed of the fastest wave, hence CFL condition.

Dispersion under PRK

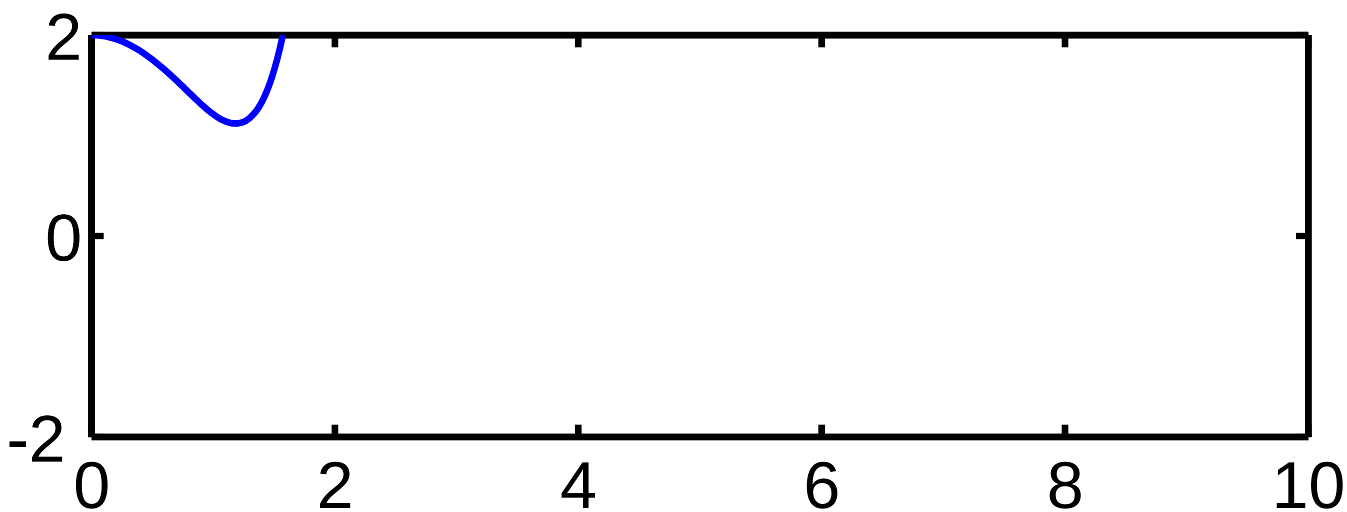
Leapfrog



Dispersion under PRK

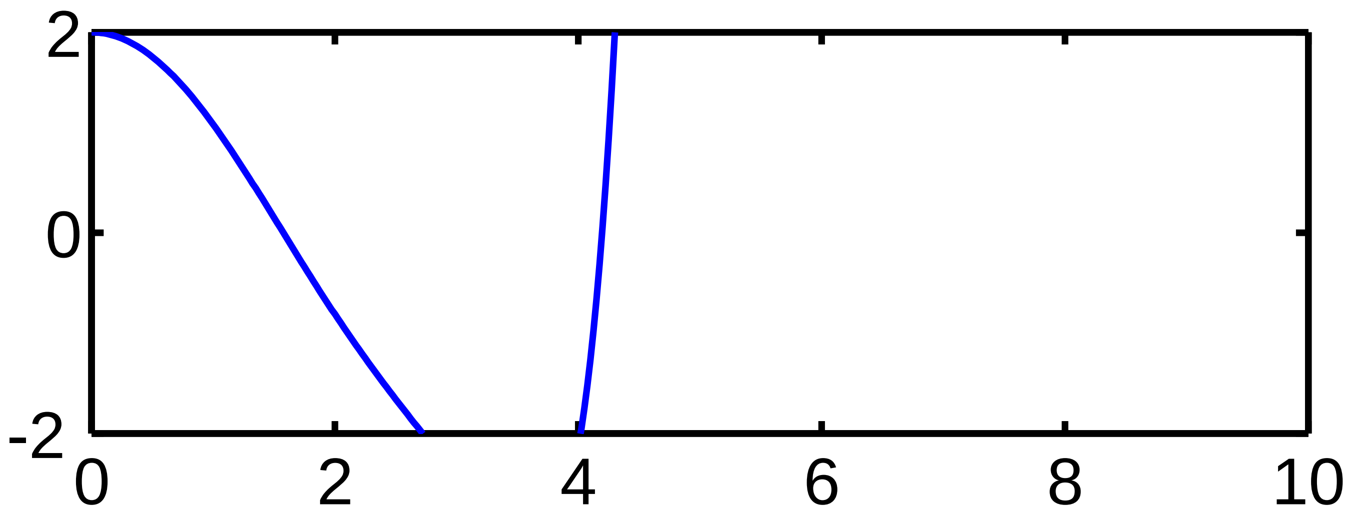
4th order composition method

$$\varphi(\alpha)\varphi((1-2\alpha)\varphi(\alpha), \quad \alpha = \frac{1}{2-2^{1/3}}$$



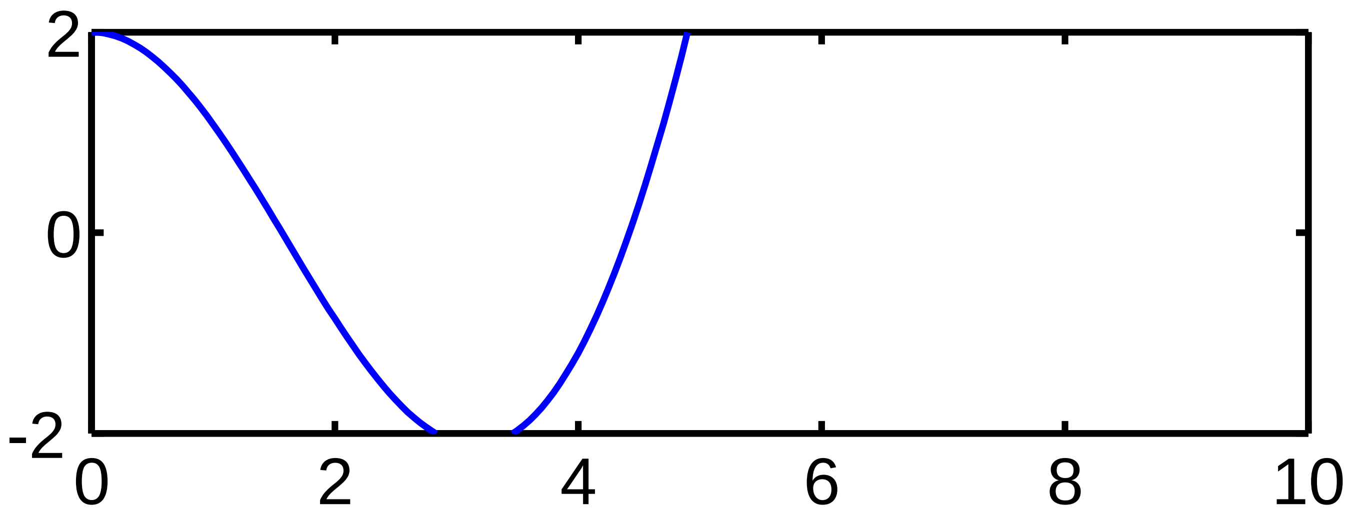
Dispersion under PRK

4th order composition method $\varphi(\alpha)^2\varphi((1-2\alpha)\varphi(\alpha)^2$,
$\alpha = \frac{1}{4-4^{1/3}}$



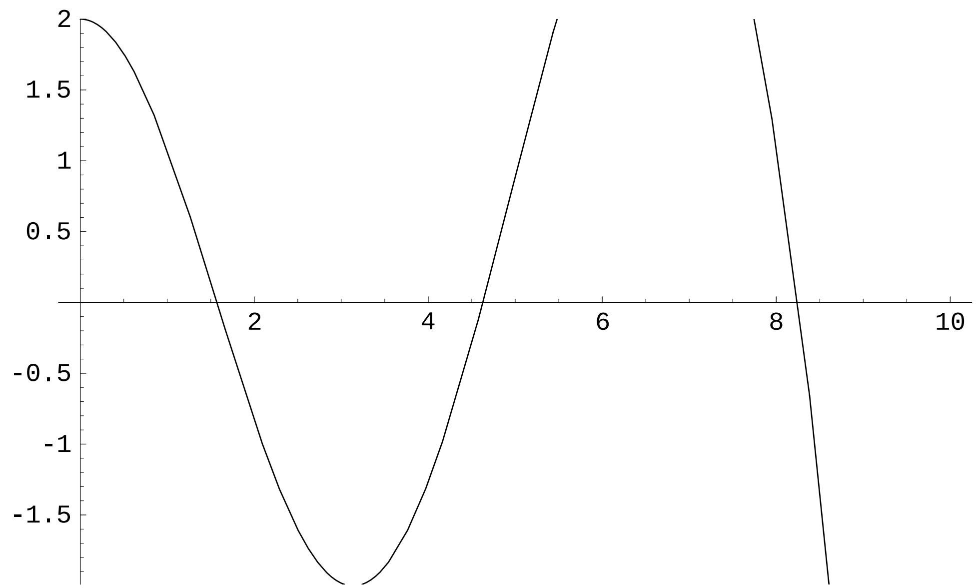
Dispersion under PRK

Lobatto $s = 3$ (but only 2 dependent variables per cell)



Dispersion under PRK

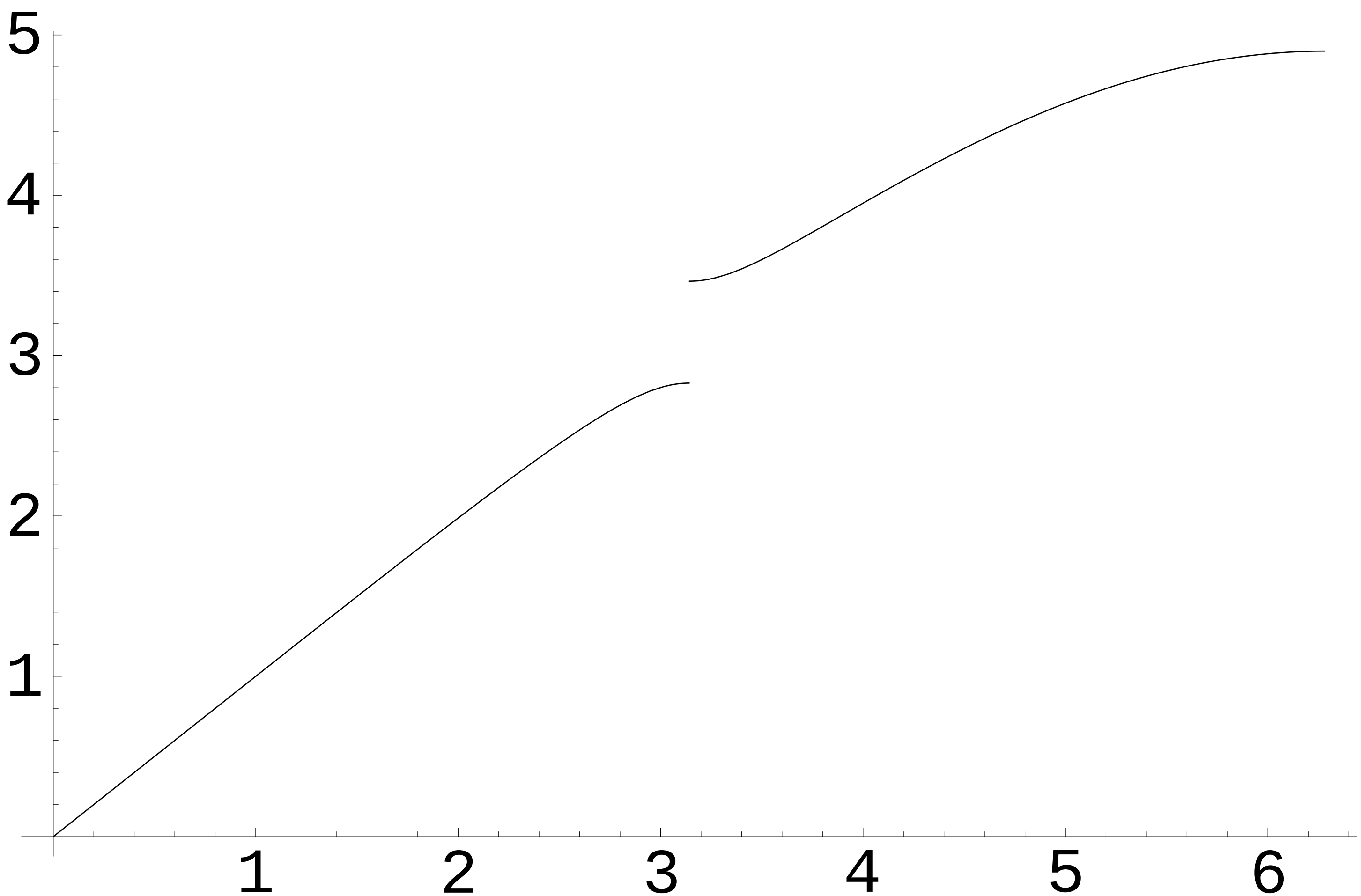
Lobatto $s = 4$



Dispersion under PRK

- The high frequency part of the dispersion relation is not captured.
- The low frequency part is captured only for sufficiently small Δx.
- The discrete dispersion relation has spurious jumps and critical points for order > 2.

Sample PRK dispersion relation



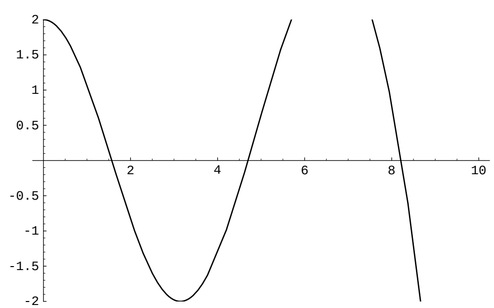
Design goals

Desirable features:

- symplectic
- symmetric
- order
- stage order
- stable
- explicit ODEs
- smooth dispersion relation

Possible new method

- Recall collocation $\Rightarrow$ symplectic PRK.
- Lobatto nodes: stage order $s-1$, explicit ODEs, discontinuous dispersion
- But $c_1 = 0$, $c_s = 1$ leads to stage order $s-1$ and explicit ODEs for any other c_j.
- Choose $c = (0, a, 1-a, 1)$.
- $a = (\sqrt{5}-5)/10 = 0.276393$ gives Lobatto method.
- $a = 0.280123$ fixes one jump in dispersion.



Order behaviour

- Dependent variables are stage values, so only get stage order
- (s for Gauss, $s - 1$ for Lobatto)
- But dispersion relation is order $2s$ (resp. $2s - 2$)!
- Can we increase the order?

Order behaviour

- Dependent variables are stage values, so only get stage order
- (s for Gauss, $s-1$ for Lobatto)
- But dispersion relation is order $2s$ (resp. $2s-2$)!
- Can we increase the order?
- Consider Lobatto IIIA–B with $s=3$.
- $Q_1 = q_0$, $Q_3 = q_1$, so leave these alone ($= q(x_j)$)
- But let $Q_2 = \mathcal{D}q(x_j + c_2\Delta x)$.
- Find that $\mathcal{D} = 1 + \frac{(\Delta x)^3}{384}\frac{\partial^3}{\partial x^3}$ increases order from 2 to 4.
- In other words, the effective order was 4.
- Output requires (approximating) $\mathcal{D}^{-1}$, but **only** on Q_2.

Order behaviour: nonlinear problems

For nonlinear problems the order $2s$ (resp. $2s-2$) is not achieved.

Requiring the same approximation $\rho = \frac{\partial}{\partial x} + h.o.t$ at each Z_j and $z_0 = z(x_0)$, $z_1 = z(x_1)$ gives

$$\mathrm{e}^{\frac{\partial}{\partial x}\Delta x} = R(\rho \Delta x)$$

and

$$Z = (I - \rho \Delta x A)^{-1} \mathbf{1} z(x_0) := \mathcal{D} z$$

Order behaviour: nonlinear problems

The ODEs are now

$$\mathbf{K}Z_t + \rho\mathbf{L}Z = \nabla S(Z).$$

Substituting for $Z = \mathcal{D}z$ in terms of the solution z to the PDE,

$$\mathcal{D}\mathbf{K}z_t + \rho\mathcal{D}\mathbf{L}z = \nabla S(\mathcal{D}z)$$

or

$$\mathbf{K}z_t + \rho\mathbf{L}z = \mathcal{D}^{-1}\nabla S(\mathcal{D}z) = \nabla S(z) + \mathcal{O}((\Delta x)^{s+1})$$

giving order $s+1$ ($s+1$ for Lobatto)
(and dispersion order $2s$ ($2s-2$ for Lobatto)

Dual roles of space and time

method	time	space
stability	$R(z)$	$R^{-1}(z)$
Gauss	order $2s$	order s
		effective order $s+1$
	implicit	implicit
	uncon. stable	uncon. stable
	speed $\to s\pi$	speed $\to \infty$
explicit PRK	explicit	unstable
implicit PRK	implicit	explicit, stable
	order $2s-2$	order $s-1$ (eff. $s+1$)
	unstable bands	dispersion jumps

The end

- Are there PRK methods in space with all desired properties?
- How bad is a discontinuous dispersion relation?
- What is the effect of the (various) multisymplectic conservation laws on the PDE and on the numerical method?

Thank you for your attention