Applications of Lie group integrators and exponential schemes

Workshop on Lie group methods and control theory,

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Brynjulf Owren

Dept of Math Sci, NTNU

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Outline

PART I (Introductory)

- Linear IVPs, Eigenvalue problems, linear PDEs
- Manifolds ("stay on manifold" principle)
- Classical problems ("curved path" principle)

PART II (Recent results on exp ints)

- A unified approach to exponential integrators
- Order theory
- Bounds for dimensions of involved function spaces

I.1 Linear IVPs

One may for instance write

$$\dot{u} = A(t)\,u, \qquad A : \mathbb{R} \rightarrow \mathbb{R}^{n \times n}$$

In literature, usually $u \in \mathbb{R}^n$.

LGI: Magnus series or related (Cayley etc)

When/Why use this scheme.

1. Highly oscillatory ODEs, large imaginary eigenvalues. Iserles
2. PDEs, $A(t)$ unbounded, classical example: Linear Schrödinger equation (LSE)). Blanes & Moan, Hochbruck & Lubich.
   Recently also Landau-Lifschitz equation Sun, Qin, Ma

I.1 Magnus works on LSE!

$$i\frac{du}{dt} = H(t)\,u, \quad H(t) \text{ unbounded, selfadjoint}$$

$d\exp_u$ is not invertible for $2k\pi i \in \sigma(u),\ k \in \mathbb{Z}\backslash\{0\}$.

Truncated series is still unbounded at ∞.
H & L find error bounds of the form

$$\|u_m - u(t_m)\| = C\,h^p\,t_m \max_{0\leq t\leq t_m} \|D^{p-1}u(t)\|$$

D is a "differentiation operator" related to the LSE.

Eigenvalue problems

Stability of travelling wave solutions to PDEs. Boils down to eigenvalue problem

$$\dot{Y} = A(t, \lambda)\, Y$$

where λ is a parameter.
Needs to be solved for several λ.

Magnus integrators used with success by Malham, Oliver and others.

Early work by Moan on such problems.

I.2 Problems on (nonlinear) manifolds

A large part of the applications I know involves the orthogonal group which acts transitively on either of

- The orthogonal group itself (or its tangent bundle).
- Stiefel manifold. ($n \times p$ matrices with orthonormal columns)
- The $n-1$-sphere. (Stiefel with $p=1$)

I.2 Orthogonal group problems

Most used examples are on $n = 3$ (3D rotations): Free rigid body, spinning top,. . .

Scheme. Most LGIs work. RKMK, Crouch-Grossmann,. . . combined with all possible “coordinates” exp, Cayley, CCSK etc.

My evaluation

- Most Lie group integrators do little else for you than maintaining orthogonality.
- Poor long-time behaviour.
- Hard to get reversible / symplectic schemes.
- There are exceptions (Lewis and Simo, Zanna et al.) but these LGIs seem expensive.

I.2 Stiefel manifolds

Some applications which involve computation on Stiefel manifolds

- Computation of Lyapunov exponents
- Multivariate data analysis (optimisation, gradient flows)
- Neural networks, Independent Component Analysis

Demands. Maintain orthonormality. Inexpensive stepping, cost $\mathcal{O}(np^2)$ per step.

Schemes. Most LGIs work. RKMK, Crouch-Grossmann,... combined with all possible "coordinates" exp, Cayley, CCSK etc. Most of them can be implemented in $\mathcal{O}(np^2)$ ops per step, but special care must be taken.

I.2 Stiefel manifolds

My evaluation

- Lie group integrators meet requirements specified in literature
- Long-time behaviour has not been an issue.
- Overall judgement: Lie group integrators are competitive, if not superior to classical integrators.

Sources

- Dieci, Van Vleck [schemes, but also general viewpoints, Lyapunov exponents]
- Trendafilov. [Multivariate data analysis]
- Celledoni, Fiori.[Neural nets, ICA]
- LGIs for Stiefel, Krogstad, Celledoni + O

I.2 Other manifold applications

- Certain PDEs whose solution evolve on (copies of) S^{n-1}, Lie group integrators have been used.
- Some special types of manifolds, e.g described by quadratic invariants like oblique manifold, DelBuono, Lopez.

I.2 Conclusions

- There are several manifold applications where Lie group integrators now represent an alternative choice. Recent research have caused implementations to be much less expensive.
- Their best feature is that they preserve the manifold. I have seen little evidence to suggest that Lie group integrators is natural for maintaining additional geometric structure. Is there hope for improvement on this point?
- The development of Lie group integrators has added important insight in the integration of DEs on manifolds. Understanding of numerics has become less dependent on specific coordinates and embeddings.

I.2 Conclusions (2)

The activity on Lie group integrators has caused progress in fields related to geometric integration:

- Computing the matrix exponential
- Computing highly oscillatory integrals
- Analysis of split-step schemes
- Exponential integrators
- Algebraic structure on trees, Hopf algebras
- Computation with the BCH-formula

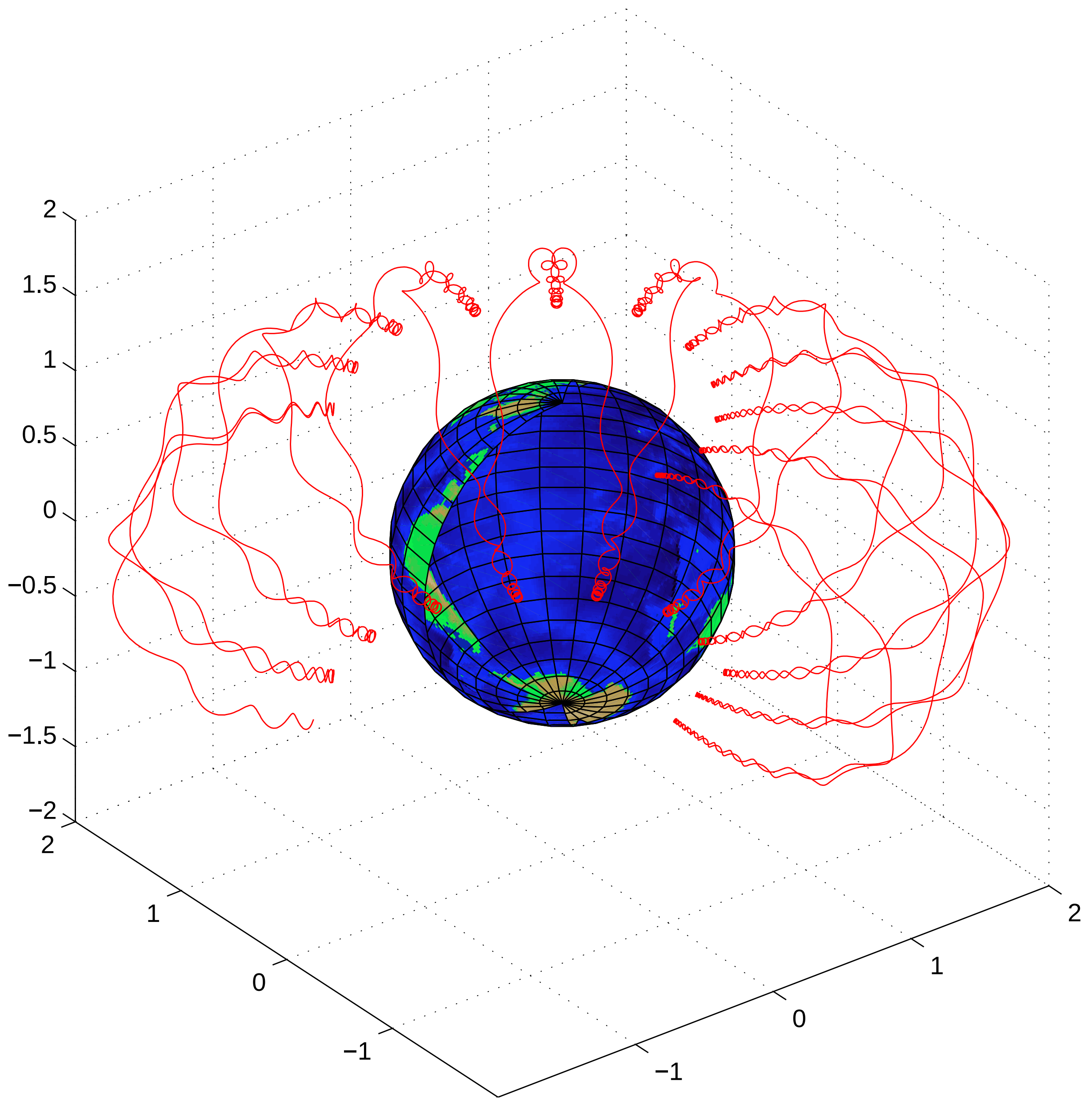
I.3 Curved path principle

- Classical numerical ODE-solvers progress solution along straight lines.
- Lie group integrators map a straight line in some other space (Lie algebra) to phase space through a nonlinear map.
- Allows for much more general “movements”.

Two excellent examples provided by Munthe-Kaas.

1. The northern light equations.
2. PDEs with perturbation terms by affine action

I.3 Northern light



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I.3, II Time Integrators for Nonlinear PDEs

Many PDEs are of the (abstract) form

$$u_t = L\,u + N(u)$$

L:	unbounded linear operator (like Δ)
$N(u)$:	a (relatively) small nonlinear term.

Includes: NLS, Nonlinear heat equations, KdV, Allen–Cahn, Kuramoto–Sivashinsky, and many more.

Unbounded L requires a form of implicit integrator.

One wants an explicit scheme for the nonlinear part.

Many time integrators are known for this purpose.

Main Classes of Time Integrators

- **LI** Linearly implicit or IMEX methods (Varah, Ruuth, Ascher, Russo and many more)
- **SS** Split step methods (Godunov, Strang etc)
- **IF** Integrating factor methods (Lawson, Nørsett)
- **SL** Sliders (Fornberg, Driscoll)
- **ETD** Exponential Time Differencing (Cox, Matthews, now also Krogstad)
- **LGI** Lie group integrators with special actions (Munthe-Kaas and others).

Exact or Rational

Among all these schemes, some use exact partial flows, others use rational approximants for the unbounded part.

Claim

Real eigenvalues of L favour rational approxmants, imaginary eigenvalues favour exact partial flows.

Henceforth we consider only schemes which apply exact partial flows (ie. “exact up to space discretization”)

Assumptions

In what follows, we shall always assume

- Whenever $L = 0$ the scheme reduces to a classical RK scheme for the problem $u_t = N(u)$
- Whenever $N(u) \equiv 0$, the exact solution of $u_t = Lu$ is recovered.

The classical Runge-Kutta scheme obtained when $L = 0$ is denoted "The underlying RK-scheme"

Our favourite choice for underlying RK scheme is the classical RK4.

Classical Runge-Kutta 4 (RK4C)

Problem of form $u_t = N(u)$. Step from t_0 to $t_0 + h$

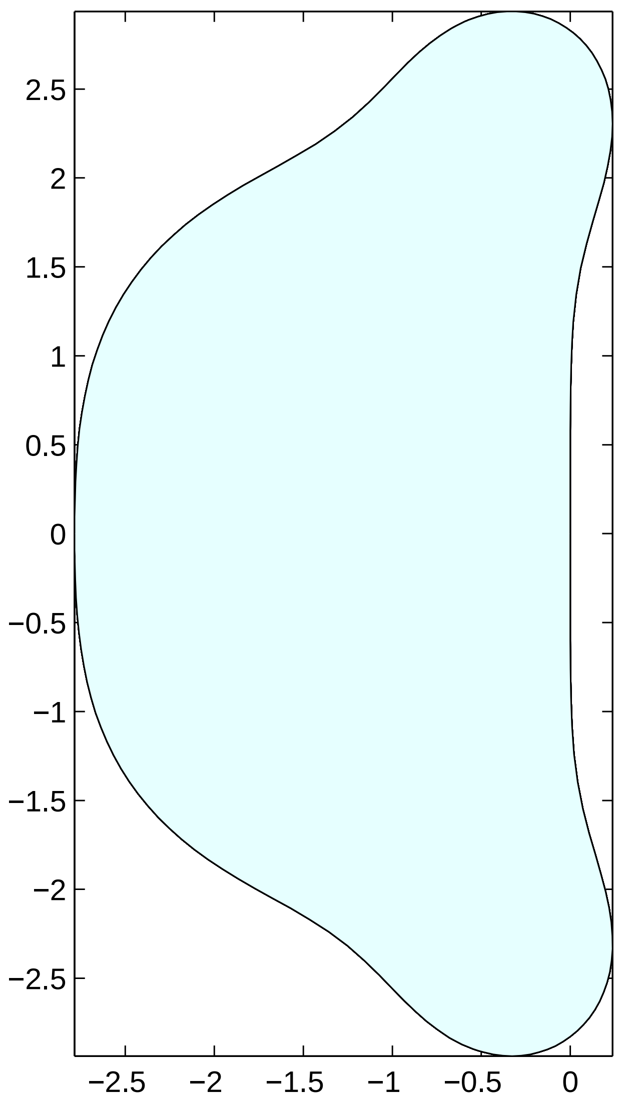
$$\mathrm{N}_1 = N(u_0)$$

$$\mathrm{N}_2 = N(u_0 + \tfrac{1}{2}h\mathrm{N}_1)$$

$$\mathrm{N}_3 = N(u_0 + \tfrac{1}{2}h\mathrm{N}_2)$$

$$\mathrm{N}_4 = N(u_0 + h\mathrm{N}_3)$$

$$u_1 = u_0 + \tfrac{h}{6}(\mathrm{N}_1 + 2\mathrm{N}_2 + 2\mathrm{N}_3 + \mathrm{N}_4)$$



An Integrating Factor Scheme (LAW4)

Lawson (1967) derived the schemes by setting

$$v(t) = \exp(-tL)u(t)$$

which leads to $v_t = \tilde{N}(v)$ where $\tilde{N} = e^{tL} \circ N \circ e^{-tL}$.
Solve resulting equation by RK4C.

$$\mathrm{N}_1 = N(u_0)$$

$$\mathrm{N}_2 = N(e^{\frac{h}{2}L}(u_0 + \tfrac{1}{2}h\mathrm{N}_1))$$

$$\mathrm{N}_3 = N(e^{\frac{h}{2}L}u_0 + \tfrac{1}{2}h\mathrm{N}_2)$$

$$\mathrm{N}_4 = N(e^{hL}u_0 + e^{\frac{h}{2}L}h\mathrm{N}_3)$$

$$u_1 = e^{hL}u_0 + \tfrac{h}{6}(e^{hL}\mathrm{N}_1 + 2e^{\frac{h}{2}L}(\mathrm{N}_2 + \mathrm{N}_3) + \mathrm{N}_4)$$

Lie Group Methods and the Affine Action

The scheme is based on the affine Lie group action.
Discrete case: Let G be a matrix group over $\mathbb{C}$ with Lie algebra $\mathfrak{g}$. Pairs $(M, b) \in G \ltimes \mathbb{C}^N$ act on points in $\mathbb{C}^N$

$$(M, b) \cdot x = Mx + b$$

The Lie algebra consists of pairs $(A, b) \in \mathfrak{g} \ltimes \mathbb{C}^N$.
Exponential map

$$\mathrm{Exp}(t(A, b)) = (e^{tA}, \frac{e^{tA} - 1}{A} b).$$

Commutator

$$[(A_1, b_1), (A_2, b_2)] = [A_1 A_2 - A_2 A_1, A_1 b_2 - A_2 b_1].$$

Here, set $\mathfrak{g} = \text{span}\{L\}$.

An RK–Munthe-Kaas Scheme (RKMK4)

From Munthe-Kaas & Owren (1999) we derive

$$\mathrm{N}_1 = N(u_0)$$

$$\mathrm{N}_2 = N(e^{\frac{hL}{2}} u_0 + \tfrac{h}{2}\phi_0(\tfrac{hL}{2})\mathrm{N}_1)$$

$$\mathrm{C}_1 = h\,L(\mathrm{N}_2 - \mathrm{N}_1)$$

$$\mathrm{N}_3 = N(e^{\frac{hL}{2}} u_0 + \phi_0(\tfrac{hL}{2})(\tfrac{h}{2}\mathrm{N}_2 - \tfrac{h}{8}\mathrm{C}_1))$$

$$\mathrm{N}_4 = N(e^{hL} u_0 + \phi_0(hL) h \mathrm{N}_3)$$

$$\mathrm{C}_2 = h\,L(\mathrm{N}_1 - 2\mathrm{N}_2 + \mathrm{N}_4)$$

$$u_1 = e^{hL} u_0 + \tfrac{h}{6}\phi_0(hL)(\mathrm{N}_1 + 2\mathrm{N}_2 + 2\mathrm{N}_3 + \mathrm{N}_4 - \mathrm{C}_1 - \tfrac{1}{2}\mathrm{C}_2)$$

where $\phi_0(z) = \frac{e^z - 1}{z}$

A Commutator-Free Lie Group Integrator, Cf4

Celledoni et al. (2002)

$$
\begin{aligned}
\mathrm{N}_1 &= N(u_0) \\
\mathrm{U}_2 &= e^{\frac{hL}{2}} u_0 + \tfrac{h}{2}\phi_0(\tfrac{hL}{2})\mathrm{N}_1 \\
\mathrm{N}_2 &= N(\mathrm{U}_2) \\
\mathrm{N}_3 &= N(e^{\frac{hL}{2}} u_0 + \tfrac{h}{2}\phi_0(\tfrac{hL}{2})\mathrm{N}_2) \\
\mathrm{N}_4 &= N(e^{\frac{hL}{2}} \mathrm{U}_2 + h\phi_0(\tfrac{hL}{2})(\mathrm{N}_3 - \tfrac{1}{2}\mathrm{N}_1)) \\
\mathrm{U}_s &= e^{\frac{hL}{2}} u_0 + \tfrac{h}{12}\phi_0(\tfrac{hL}{2})(3\mathrm{N}_1 + 2\mathrm{N}_2 + 2\mathrm{N}_3 - \mathrm{N}_4) \\
u_1 &= e^{\frac{hL}{2}} \mathrm{U}_s + \tfrac{h}{12}\phi_0(\tfrac{hA}{2})(-\mathrm{N}_1 + 2\mathrm{N}_2 + 2\mathrm{N}_3 + 3\mathrm{N}_4)
\end{aligned}
$$

A Cox and Matthews Scheme (C-M4)

This scheme has the same $\mathrm{N}_1, \ldots, \mathrm{N}_4$ as Cf4.

$$u_1 = e^{hA}u_0 + h(f_2(hL)\mathrm{N}_1 + 2f_3(hL)(\mathrm{N}_2 + \mathrm{N}_3) + f_4(hL)\mathrm{N}_4)$$

where

$$f_2(z) = \frac{-4 - z + e^z(4 - 3z + z^2)}{z^3}$$

$$f_3(z) = \frac{2 + z + e^z(-2 + z)}{z^3}$$

$$f_4(z) = \frac{-4 - 3z - z^2 + e^z(4 - z)}{z^3}$$

Derivation technique: Unknown!

A unified format

By carefully studying all these schemes, one finds that they all fit into the framework

$$N_r = N(e^{c_r hL}\, u_0 + h \sum_{j=1}^{s} a_r^j(hL)\, N_j), \quad r = 1, \ldots, s$$

$$u_1 = e^{hL}\, u_0 + h \sum_{r=1}^{s} b^r(hL)\, N_r.$$

$$a_r^j(z) = \sum_m \alpha_r^{j,m}\, z^m, \quad b^r(z) = \sum_m \beta^{r,m}\, z^m$$

$(\alpha_r^{j,0}),\ (\beta^{r,0})$ underlying RK scheme.

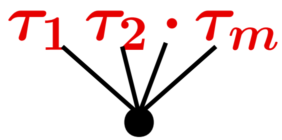
Order theory

Order conditions and B-series can be derived by standard tools (rooted trees).

T : The set of bicolored rooted trees where each white node has at most 1 child.

T' : Subset of T where each white node has precisely one child (no white leaves)

$W_+ : \tau \quad \mapsto$ 

, $\qquad B_+ : \{\tau_1, \ldots, \tau_m\} \quad \mapsto$ 

- B-series indexed by T.
- Order conditions: T' suffices.

Order conditions for exponential integrators

An exponential integrator has order p if

$$\mathbf{u}_1(\tau) = \frac{1}{\gamma(\tau)}, \quad \text{for all } \tau \in T' \text{ such that } |\tau| \leq p,$$

where

$$\mathbf{u}_1(\emptyset) = \mathrm{U}_r(\emptyset) = 1, \; 1 \leq r \leq s,$$

$$\mathbf{u}_1(W_+^m B_+(\tau_1, \ldots, \tau_\mu)) = \sum_r \beta^{r,m} \mathrm{U}_r(\tau_1) \cdots \mathrm{U}_r(\tau_\mu)$$

$$\mathrm{U}_r(W_+^m B_+(\tau_1, \ldots, \tau_\mu)) = \sum_j \alpha_r^{j,m} \mathrm{U}_j(\tau_1) \cdots \mathrm{U}_j(\tau_\mu)$$

Number of conditions

Generating function for $\#$ trees with q nodes in T'

$$M(x) = \frac{x}{1-x}\,\exp\left(M(x) + \frac{M(x^2)}{2} + \frac{M(x^3)}{3} + \cdots\right)$$

The number of order conditions for each order 1 to 9 is $1, 2, 5, 13, 37, 108, 332, 1042, 3360$.

Coefficient function spaces

$a_r^j(z),\ b^r(z)$ belong to some function spaces we denote $V_a,\ V_b$ of finite dimension.
Often, $V_a,\ V_b$ they are related to the functions

$$\phi_k(z) = \int_0^1 e^{(1-\theta)z}\,\theta^k\,d\theta, \quad \text{e.g.} \quad \phi_0(z) = \frac{e^z - 1}{z}$$

Scheme	V_a	V_b
Cf4	$\phi_0(\frac{z}{2}),\ z\phi_0(\frac{z}{2})^2$	$\phi_0(\frac{z}{2}),\ \phi_0(z)$
C-M4	As Cf4	$\phi_0(z),\ \phi_1(z),\ \phi_2(z)$
RKMK4:	$\phi_0(\frac{z}{2}),\ z\phi_0(\frac{z}{2})$	$\phi_0(z),\ z\phi_0(z)$
Law4:	$1,\ e^{z/2}$	$1,\ e^{z/2},\ e^z$

Assumption and bounds

Let V of dim K be a function space as above.
Assumption. The map

$$f \in V \mapsto (f(0), f'(0), \dots, f^{(K-1)}(0)) \in \mathrm{R}^K$$

is injective

Theorem. For any pth order exponential integrator, one has

$$K_a = \dim V_a \geq \left\lfloor \frac{p}{2} \right\rfloor, \qquad K_b = \dim V_b \geq \left\lfloor \frac{p+1}{2} \right\rfloor.$$

Moreover, the lower bound for V_b is always attainable with basis $\phi_0, \dots, \phi_{K_b-1}$

Remarks

- We have no general proof that lower bound for K_a is sharp. However, with $p = 5$ one can use $K_b = 2$ with $\phi_1(z), \phi_1(\frac{3}{5}z)$.
- A procedure for constructing exponential integrators has been developed. One starts with an arbitrary underlying scheme as well as V_a, V_b.
- The really interesting part is still ahead: Choose spaces V_a, V_b to deal with unbounded L. In the time to come, we focus in particular on the NLS.

Natural Continuous Extensions Zennaro 1986

Let $(\alpha_r^{j,0})$ $(\beta^{r,0})$ define an underlying Runge-Kutta scheme of order p

Suppose that polynomials $w_1(\theta), \ldots, w_s(\theta)$ of degree d can be found such that

$$\bar{N}(t_0 + \theta h) := \sum_r w_r'(\theta)\, \mathrm{N}_r$$

satisfies

$$\max_{t_0 \le t \le t_1} |N(u(t)) - \bar{N}(t)| = \mathcal{O}(h^{d-1})$$

$$\int_{t_0}^{t_1} G(t)(N(u(t)) - \bar{N}(t))\, dt = \mathcal{O}(h^{p+1})$$

NB! Requires $a_r^j(z)$ to be given.

NCEs continued

Replace $u_t = L\,u + N(u)$ by $v_t = L\,v + \bar{N}(t)$, solve exactly, and set $u_1 := v(h)$. Yields exponential integrator of order p with

$$b^r(z) = \int_0^1 \exp((1-\theta)z)w_r'(\theta)\,d\theta$$

$$= \beta^{r,0} + z\int_0^1 \exp((1-\theta)z)w_r(\theta)\,d\theta$$

In particular, these are expressed in terms of

$$\phi_k(z) = \int_0^1 \exp(z(1-\theta))\,\theta^k\,d\theta,\ k = 0, 1, \ldots$$

We have rediscovered the Cox& Matthews schemes.

Why it works

$$
\begin{aligned}
(u-v)_t &= L(u-v) + (N(u) - \bar{N}(t)) \\
&\Downarrow \\
(u-v)(t_1) &= \int_{t_0}^{t_1} e^{(t_1-t)L}(N(u(t) - \bar{N}(t))\, dt \\
&= \mathcal{O}(h^{p+1})
\end{aligned}
$$

thanks to the definition of NCEs

Theorem of Zennaro

The following result gives us a sharp lower bound for the number of ϕ_k functions which must be included

Any NCE satisfies

$$q := \left[\frac{p+1}{2}\right] \leq d \leq \min\{p, s^*\}.$$

Moreover, and NCE of degree q always exists.

Conclusion. An underlying RK scheme of order p can always be extended to an exponential integrator of order p where

$$b^r(z) \in \text{span}\{\phi_0, \ldots, \phi_{q-1}\}, \ \forall r$$

The nonlinear Schrödinger equation

Generally

$$iu_t = -\Delta u + \left(V(x) + \lambda |u|^{2\sigma}\right) u, \quad (t, x) \in \mathbb{R} \times \mathbb{R}^d$$

Here

$$0 < \sigma, \quad \text{and} \quad \sigma < \frac{2}{d-2} \quad \text{if} \quad d \geq 3.$$

- Potential: $V(x) \in L_1 + L_\infty$.
- IC: $u(x, 0) = u_0 \in \Sigma \subset H^1$.
- Here, let $d = 1$ and $(x, t) \in S^1 \times \mathbf{R}$.
- Usually, take $\sigma = 1$ (cubic case).

Spectral Discretisation in Space

Use $2n$ modes and set

$$c^k(t) = \sum_{m=-n}^{n-1} U(\tfrac{2m\pi}{2n}, t) e^{-imk}$$

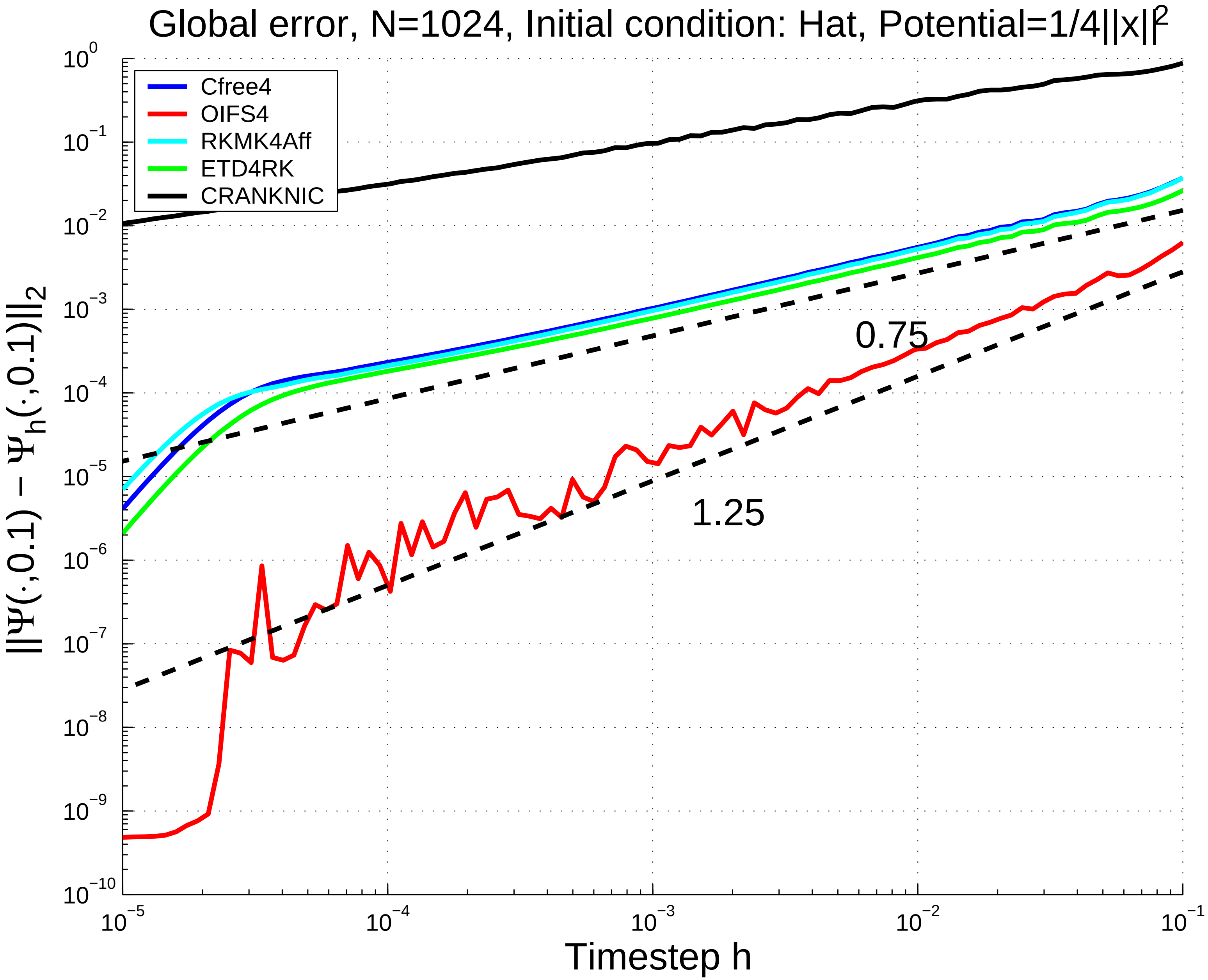
leading to the NLS spectrally discretised system

$$\frac{\mathrm{d}c}{\mathrm{d}t} = D\,c + \mathcal{F}_n \circ \check{\mathrm{N}} \circ \mathcal{F}_n^{-1}(c)$$

$$D = \mathrm{diag}(-ik^2)_{k=-n}^{n-1}$$

$$i\check{\mathrm{N}}(U)_\ell = (V(x_\ell) + \lambda |U(x_\ell)|^2) U(x_\ell).$$

NumExp 1


Global error, N=1024, Initial condition: Hat, Potential=1/4||x||2
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
0.75
1.25
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h

A Simplified Case

Let us

- Focus on one scheme, say the Cf4 scheme.
- For analysis, set $V(x) \equiv v$ and $\lambda = 0$.

In this case, the SDNLS decouples into scalar equations

$$\dot{c}^k = \alpha_k c^k + \beta^k$$

where $\alpha_k = -ik^2$, and $\beta = -iv$.

Setting $a_k = \frac{\beta}{\alpha_k}$, $m_k = e^{-\frac{i}{2}hk^2}$ the Cf4 scheme is

$$c_1 = p(m_k, a_k)c_0, \quad p(m, a) = \sum_{j=0}^{5} r_j(a)m^j, \quad r_j \in \Pi_4[a]$$

Global Error Cf4

Need to find global error at $t = T$.
Must estimate $|p_k^n - e_k^n|$ where $n = T/h$

$$p_k = p(m_k, a_k), \; e_k = \exp(-ih(k^2 + v))$$

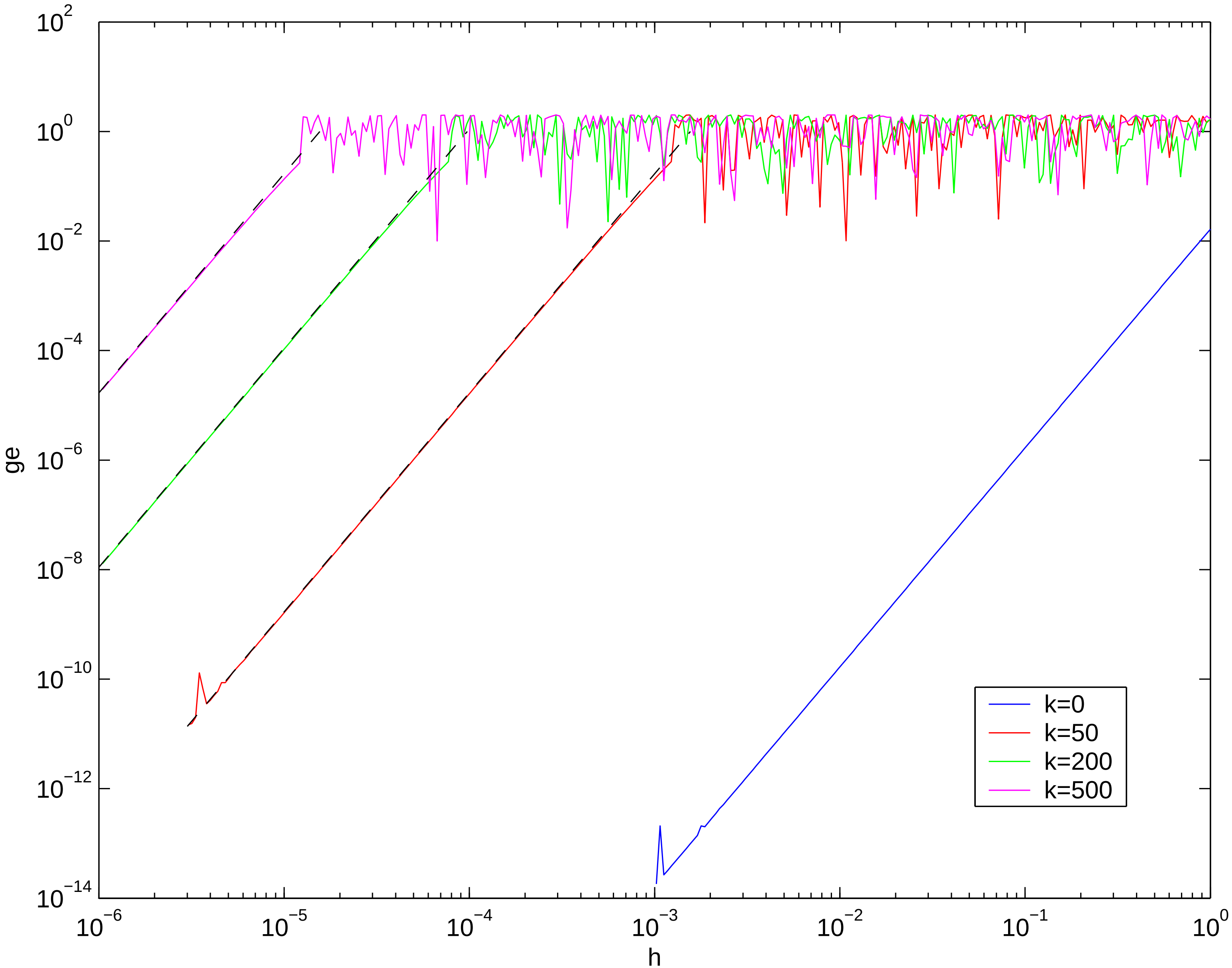
A rigorous analysis shows that up to leading order

$$|p_k^n - e_k^n| \approx \left(\frac{hk^2}{S_b}\right)^4, \quad S_b = \left(\frac{480}{T|v|}\right)^4$$

whenever $hk^2 \ll 1$ whereas for $hk^2 \gg 1$ (and $|v| \leq \frac{1}{2}k^2$)

$$|p_k^n - e_k^n| \leq 2$$

The Global Error for Decoupled Case



Summing It Up

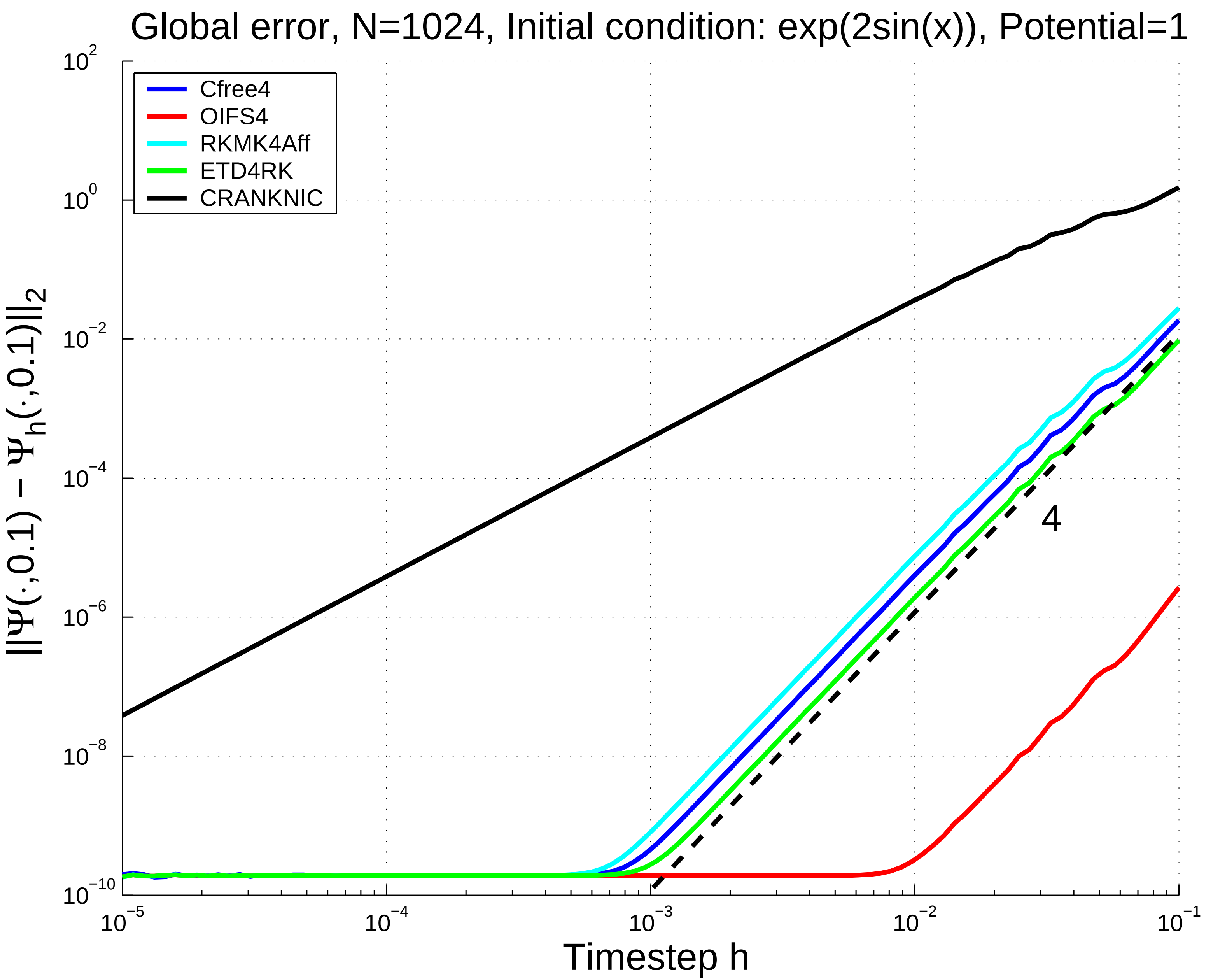
The ℓ_2-norm of the global error is found by summing up

$$\|\mathrm{ge}\|^2 = \sum_k |p_k^n - e_k^n|^2 \, |c_0^k|^2.$$

We may assume that $|c_0^k| \leq \frac{K_0}{k^p}$ (holds in particular if u_0 is $C^p(S^1, \mathbb{C})$). Assuming that $N^2 h \gg 1$ we estimate by Euler–Maclaurin's formula

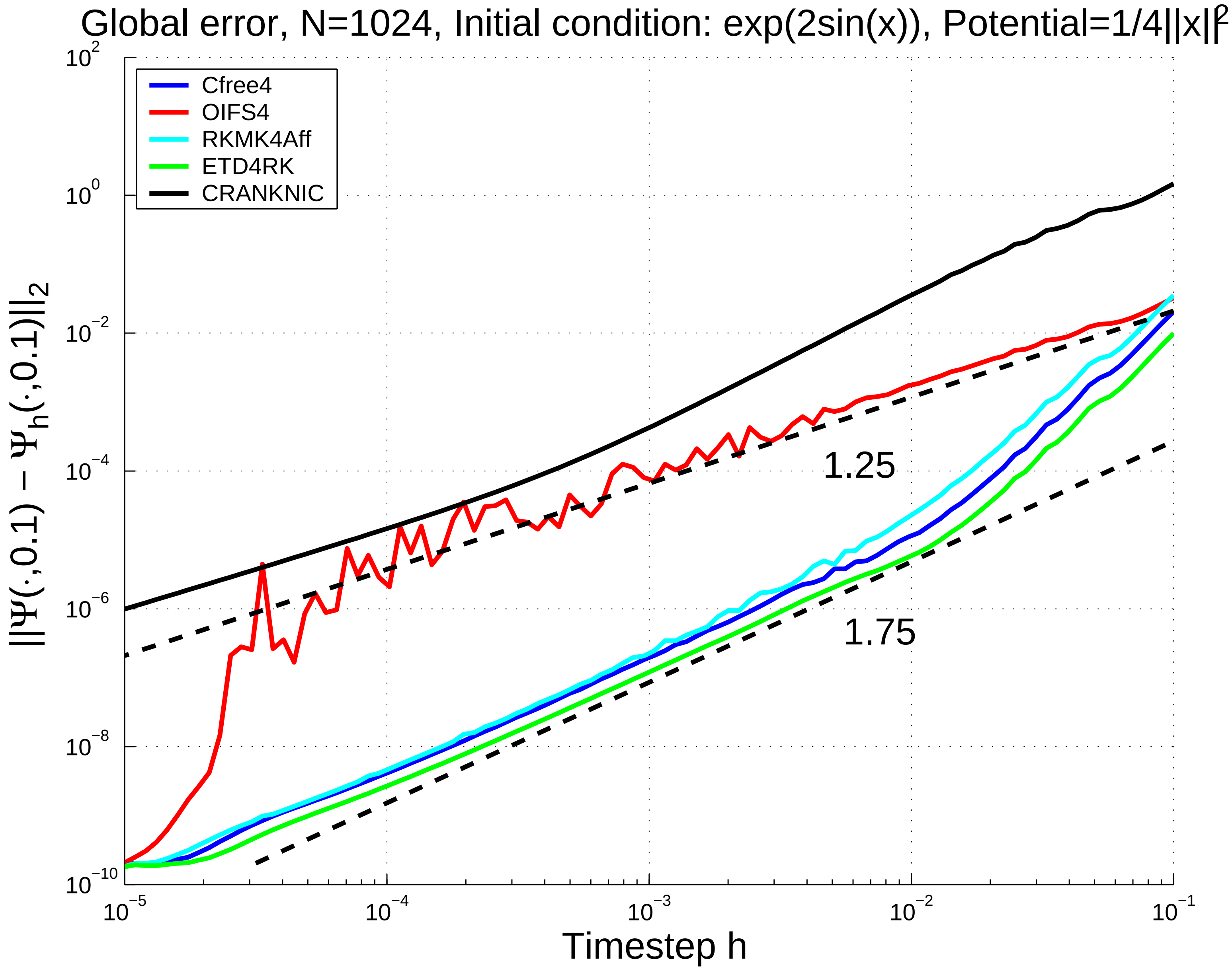
$$\|\mathrm{ge}\| \approx C\, h^{\frac{2p-1}{4}}, \quad p \leq 8.$$

Figure 1



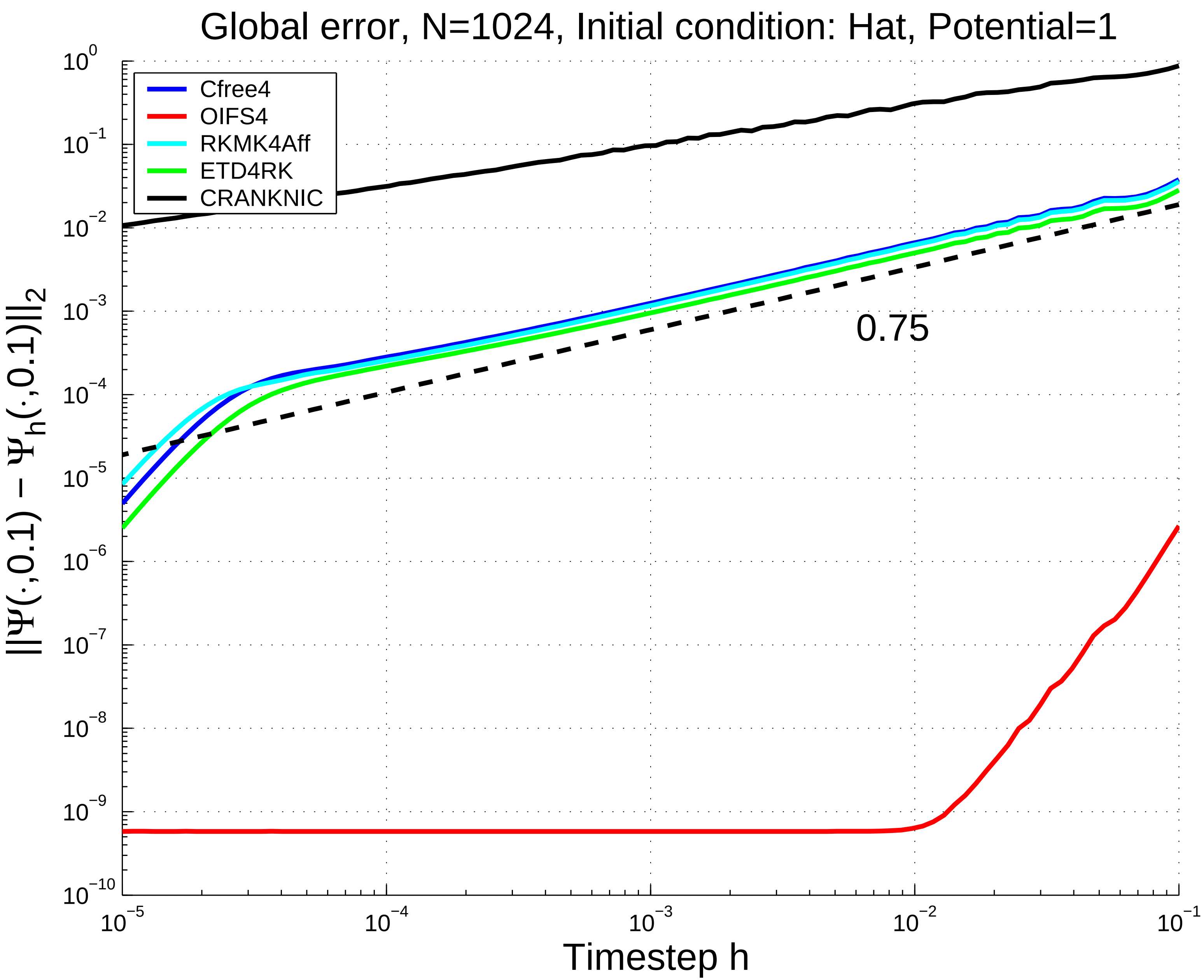
Global error, N=1024, Initial condition: exp(2sin(x)), Potential=1
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
4
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
Timestep h
$||\Psi(\cdot,0.1) - \Psi_h(\cdot,0.1)||_2$

Figure 2



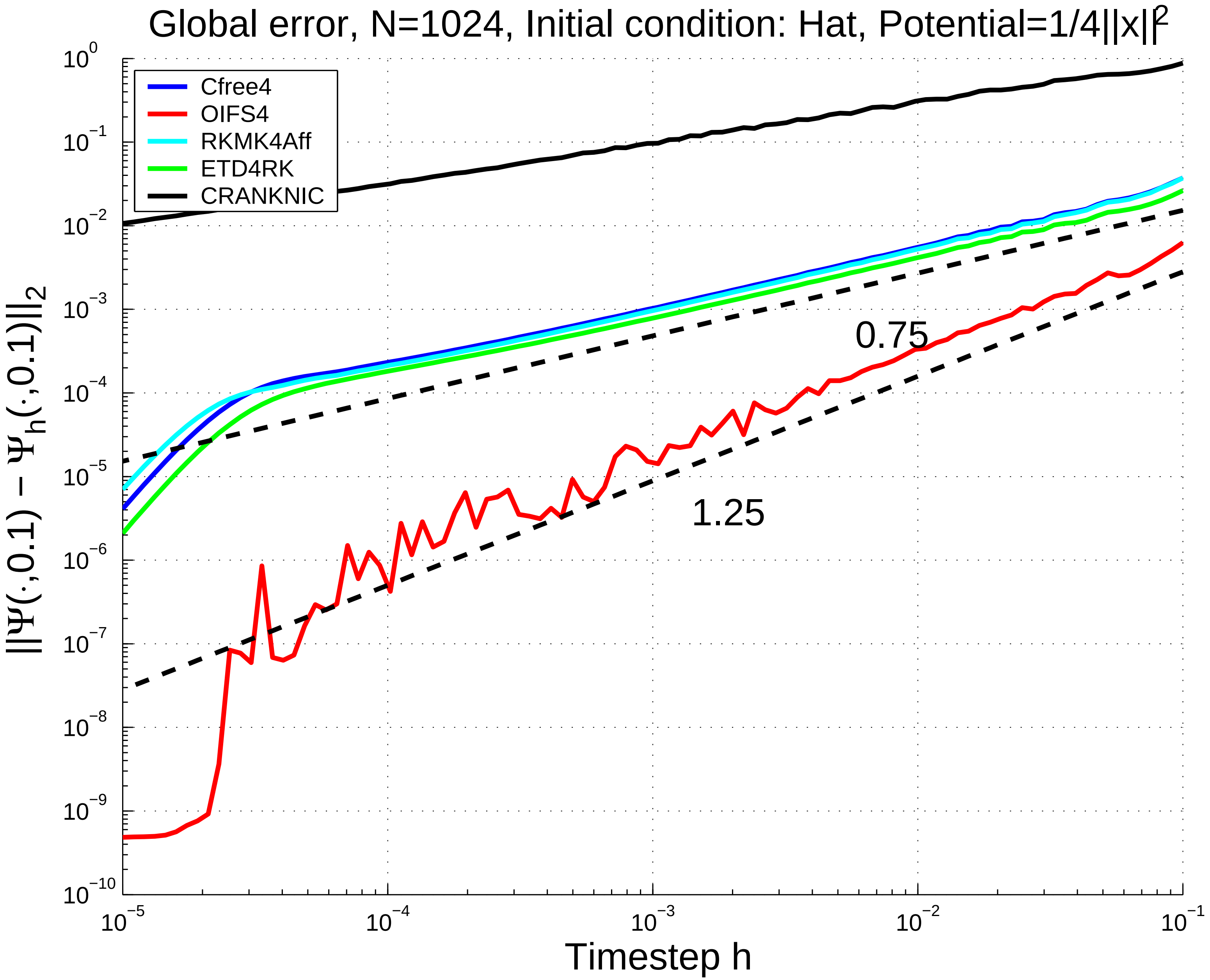
Global error, N=1024, Initial condition: exp(2sin(x)), Potential=1/4||x||²
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
1.25
1.75
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h

Figure 3



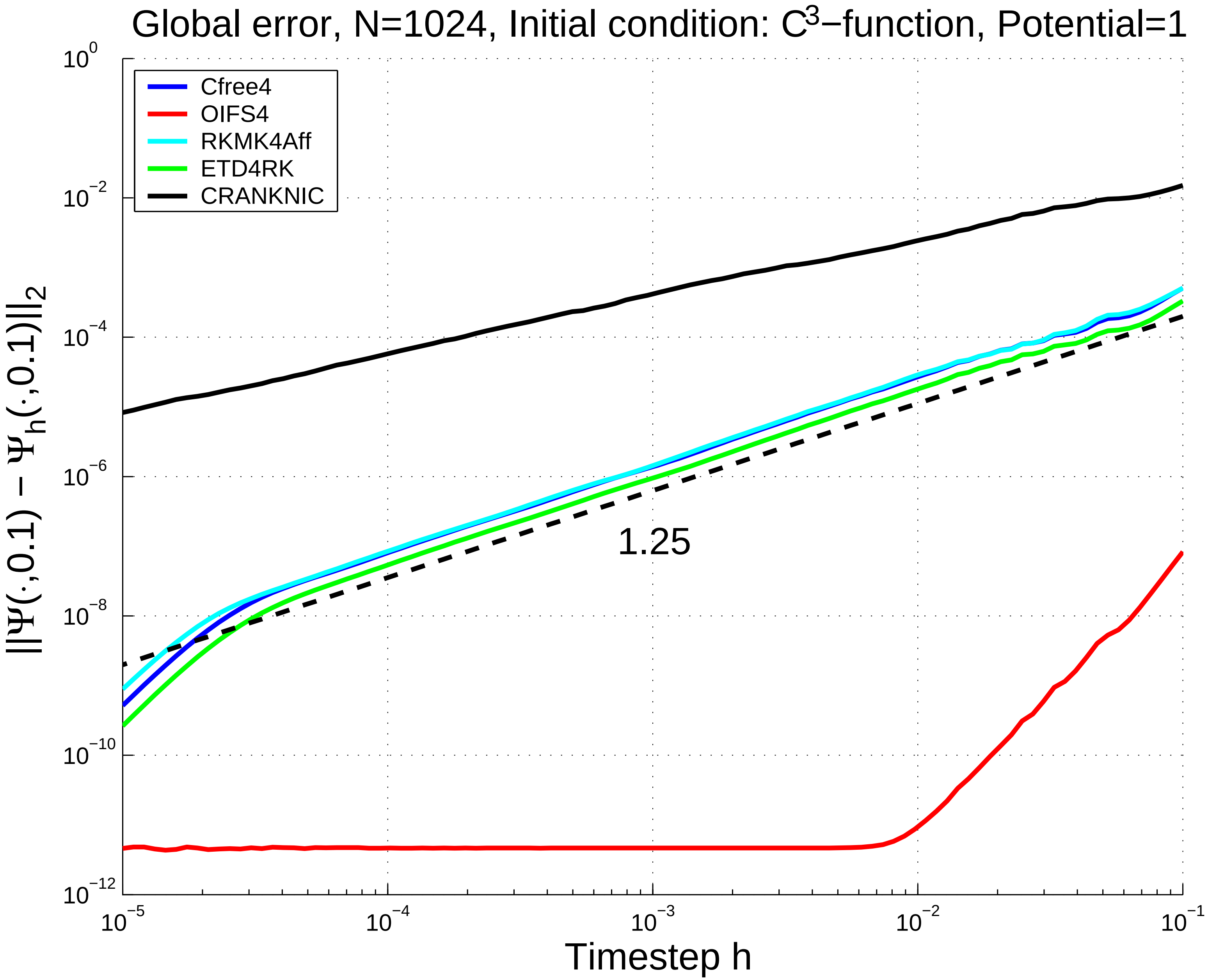
Global error, N=1024, Initial condition: Hat, Potential=1
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
0.75
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
$||\Psi(\cdot,0.1) - \Psi_h(\cdot,0.1)||_2$
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
Timestep h

Figure 4



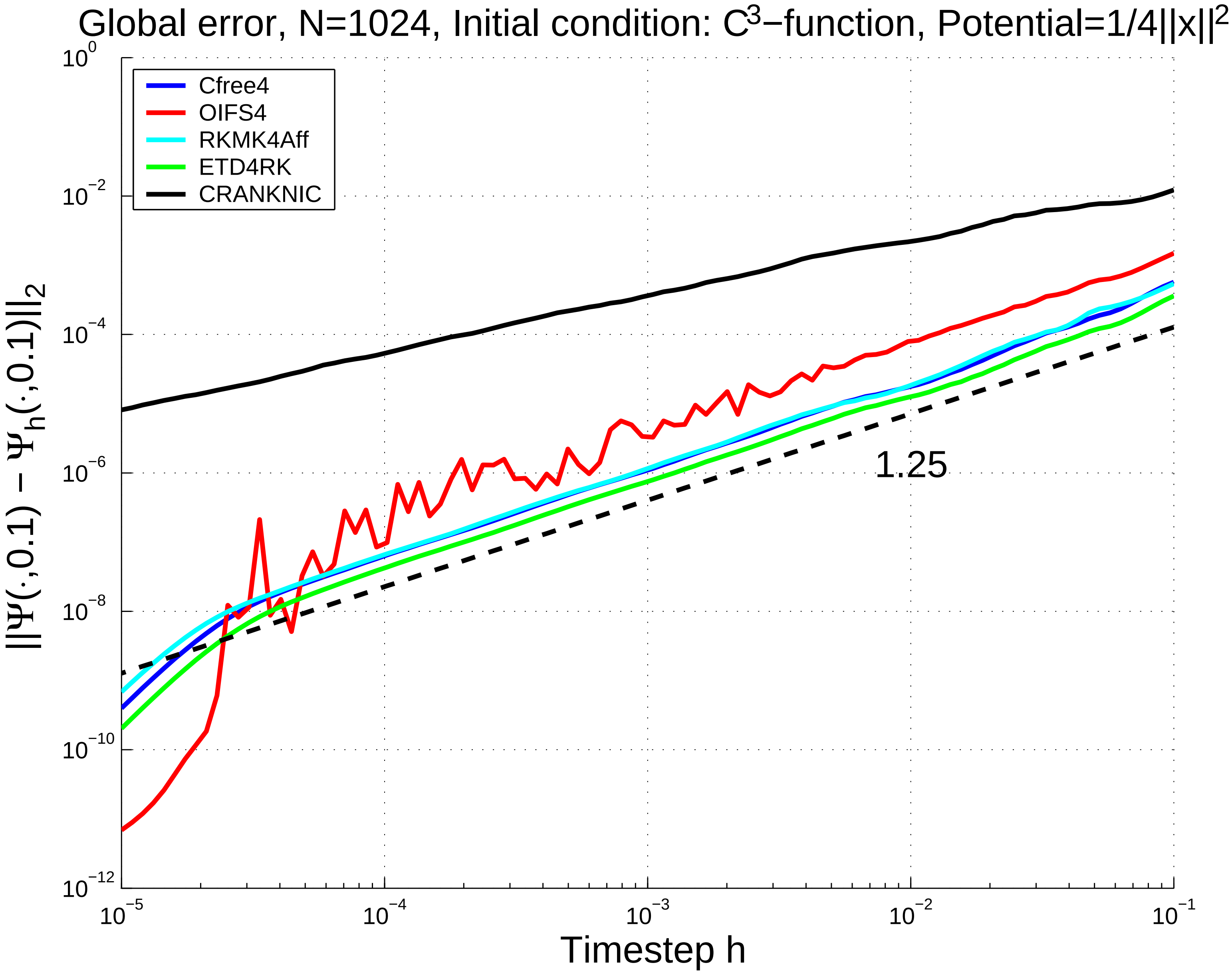
Global error, N=1024, Initial condition: Hat, Potential=1/4||x||2
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
0.75
1.25
10^0
10^−1
10^−2
10^−3
10^−4
10^−5
10^−6
10^−7
10^−8
10^−9
10^−10
10^−5
10^−4
10^−3
10^−2
10^−1
Timestep h
||Ψ(·,0.1) − Ψh(·,0.1)||2

Figure 5



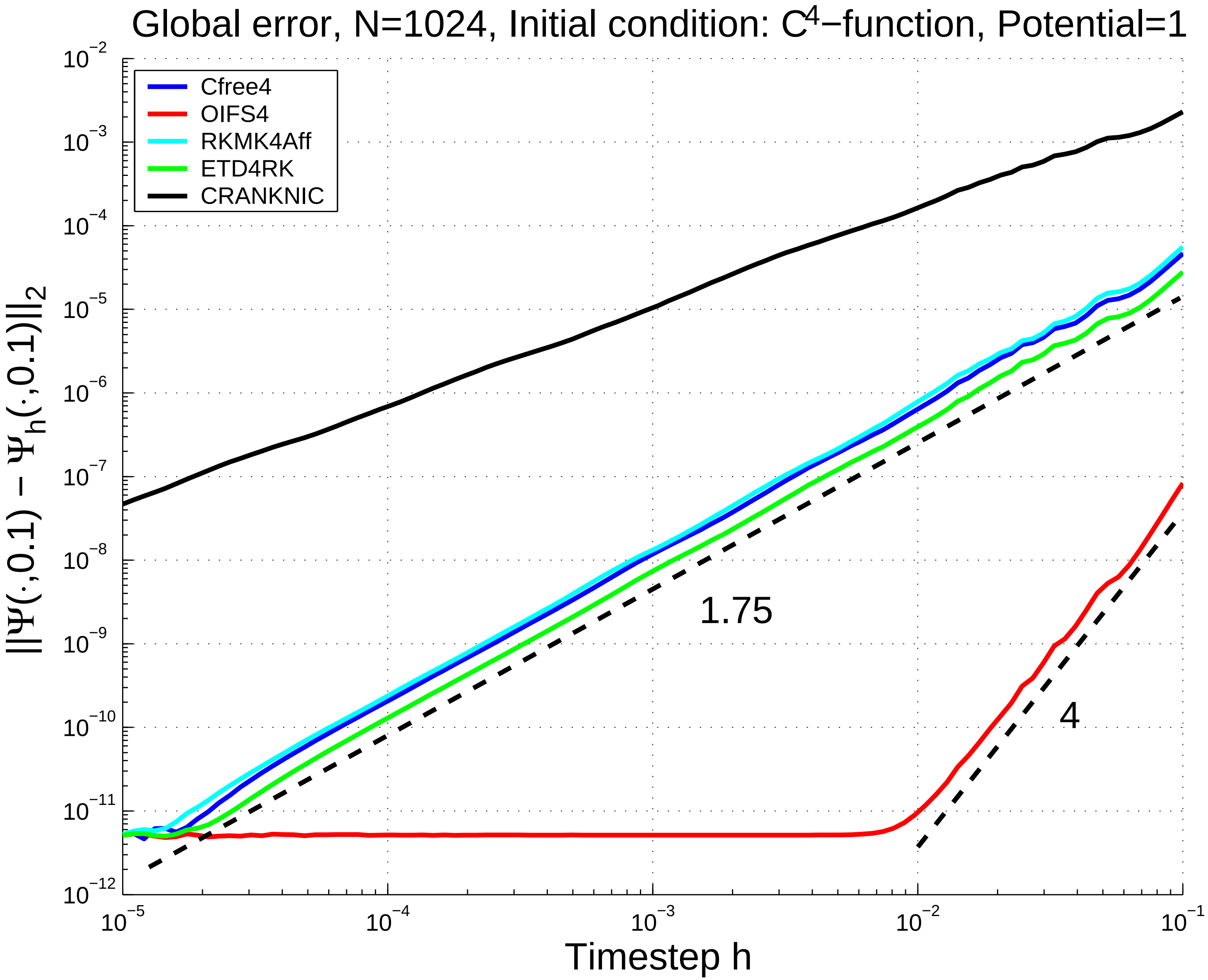
Global error, N=1024, Initial condition: C3−function, Potential=1
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
1.25
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−5
10^−4
10^−3
10^−2
10^−1

Figure 6



Global error, N=1024, Initial condition: C3−function, Potential=1/4||x||2
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
1.25
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−5
10^−4
10^−3
10^−2
10^−1

Figure 7



Global error, N=1024, Initial condition: C4−function, Potential=1
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
1.75
4
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h
10−2
10−3
10−4
10−5
10−6
10−7
10−8
10−9
10−10
10−11
10−12
10−5
10−4
10−3
10−2
10−1

Figure 8

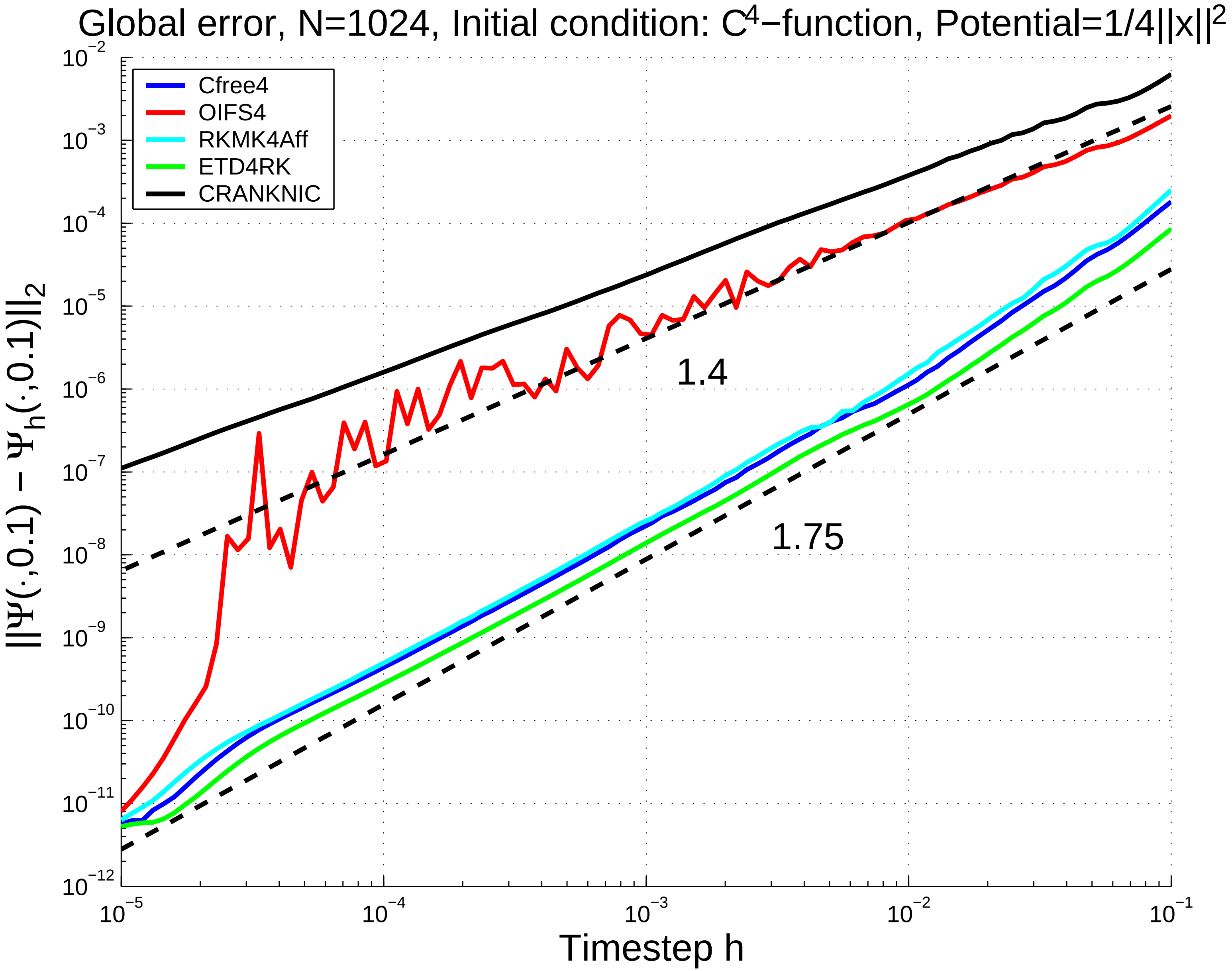

Global error, N=1024, Initial condition: C^4−function, Potential=1/4||x||^2
$||\Psi(\cdot,0.1) - \Psi_h(\cdot,0.1)||_2$
Timestep h
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
1.4
1.75
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
10^{-1}

Figure 9

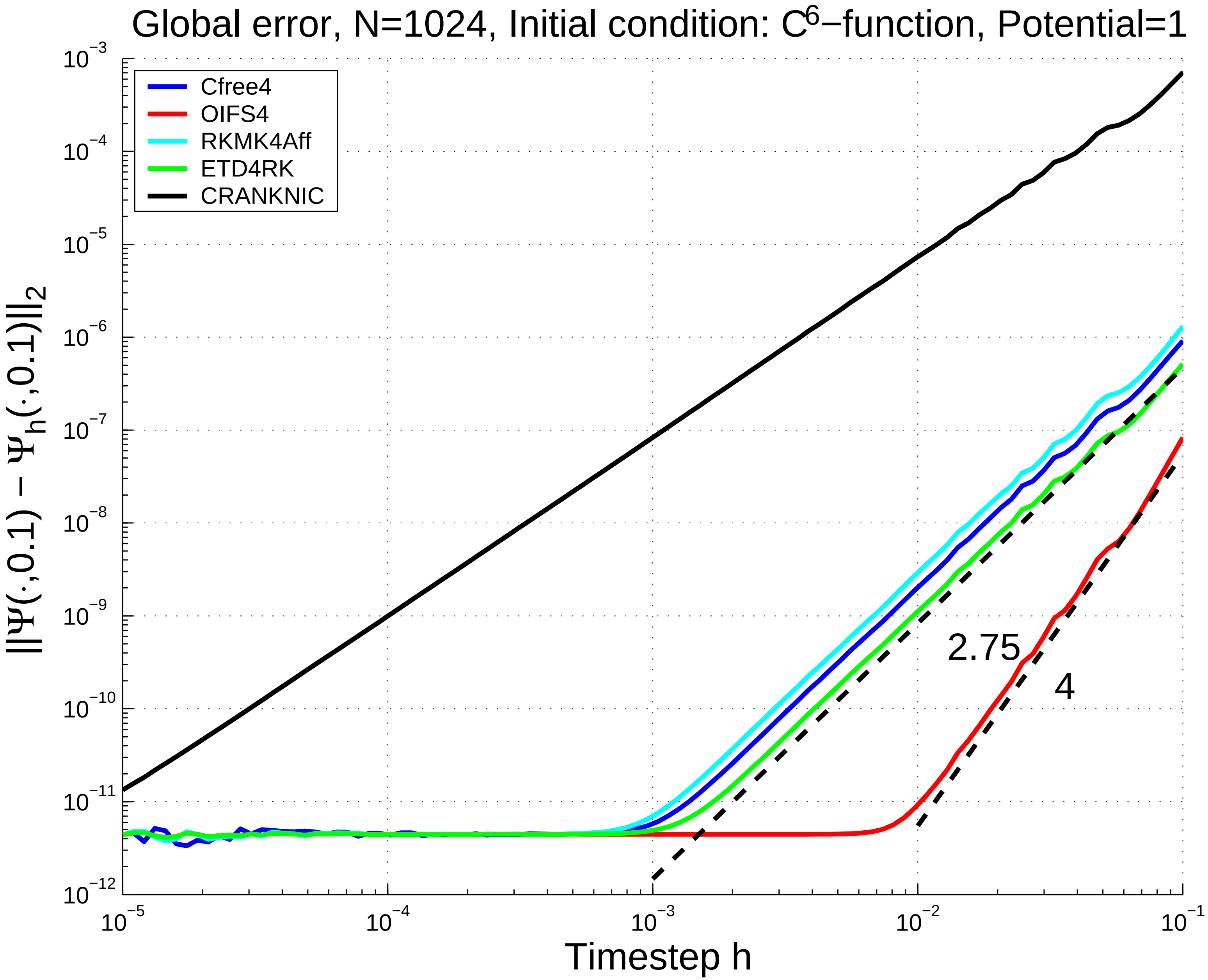
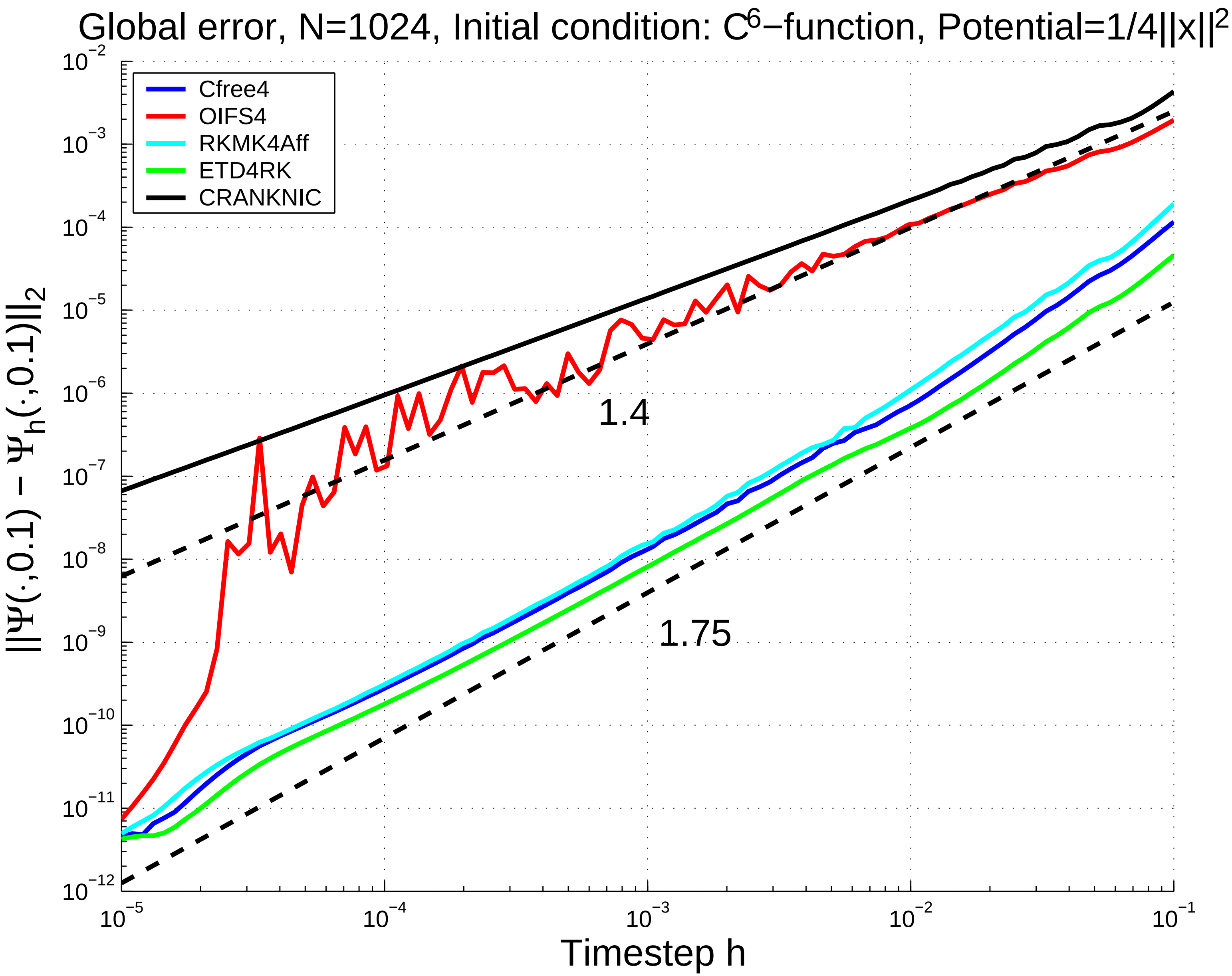

Global error, N=1024, Initial condition: C6−function, Potential=1
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
2.75
4
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h
10−3
10−4
10−5
10−6
10−7
10−8
10−9
10−10
10−11
10−12
10−5
10−4
10−3
10−2
10−1

Figure 10



Global error, N=1024, Initial condition: C6−function, Potential=1/4||x||2
Cfree4
OIFS4
RKMK4Aff
ETD4RK
CRANKNIC
1.4
1.75
||Ψ(·,0.1) − Ψh(·,0.1)||2
Timestep h

Our Work Plan

- Do this analysis for the other schemes
- Extend to more general $V(x)$
- Can the analysis include the nonlinear term? Numerical tests show that it has little impact.
- We want to do the semiclassical case
- More space dimensions, more general boundary conditions
- Compare results with those from geometric integrators

Long Time Integration

For systems with a symplectic structure, experience shows that retention of such a structure in the numerical scheme enhances the long time quality of integration. Consider (Islas et al) the following 1D nonlinear Schrödinger equation

$$iu_t = -u_{xx} - 2|u|^2 u$$

on the circle. It is a completely integrable Hamiltonian system in the variables (q, q^*) with

$$H(q, q^*) = i \int_0^L (|q|^4 - |q_x|^2)\,\mathrm{d}x$$

$$\omega = \int_0^L (\mathrm{d}q^* \wedge \mathrm{d}q)\,\mathrm{d}x$$

Possible Strategies

1. Find a multisymplectic structure Reich (2000) and discretise simultaneously in space and time to preserve this structure.
2. Introduce an integrable space discretization (Ablowitz/Ladik), the resulting ODE system is not canonical. So standard symplectic integrators cannot be used, one may then
   (a) Use a Lie–Poisson type integrator based on the generating function technique
   (b) Apply (locally) the Darboux transformation to obtain a standard canonical Hamiltonian system to which a symplectic scheme can be applied

A Multisymplectic Structure

The above Schrödinger equation can be written in the form

$$\mathrm{M}z_t + \mathrm{K}z_x = \nabla_z S(z), \quad z \in \mathbb{R}^4.$$

Here M and K are skew-symmetric 4×4-matrices, and $S : \mathbb{R}^4 \to \mathbb{R}$.

The two matrices define symplectic structures ω, κ on $\mathbb{R}^{\mathrm{rank(M)}}$ and $\mathbb{R}^{\mathrm{rank(K)}}$.

$$\omega(U, V) = V^T \mathrm{M} U, \quad \kappa(U, V) = V^T \mathrm{K} U.$$

In NLS we let $a = \mathrm{Re}\, u$, $b = \mathrm{Im}\, u$, $z = (a, b, a_x, b_x)^T$ so

$$S(z) = \tfrac{1}{2}(a_x^2 + b_x^2 + (a^2 + b^2)^2).$$

Multisymplectic Cont'd

Let U, V be two solutions of the variational equation

$$\mathrm{M}\mathrm{d}z_t + \mathrm{K}\mathrm{d}z_x = \mathrm{D}_{zz}S(z)\mathrm{d}z$$

It easily follows that this pair of solutions satisfies

$$\partial_t \omega(U, V) + \partial_x \kappa(U, V) = 0$$

the symplectic conservation law.
The simplest multisymplectic scheme is obtained as the concatenated midpoint rule:

$$\mathrm{M}\left(\frac{z_{i+\frac{1}{2}}^{j+1} - z_{i+\frac{1}{2}}^{j}}{\Delta t}\right) + \mathrm{K}\left(\frac{z_{i+1}^{j+\frac{1}{2}} - z_{i}^{j+\frac{1}{2}}}{\Delta x}\right) = \nabla_z S\left(z_{i+\frac{1}{2}}^{j+\frac{1}{2}}\right)$$

The Ablowitz–Ladik Truncation

For simplicity, set $q = u$ and $p = u^*$. The above NLS now has the formulation

$$iq_t = -q_{xx} - 2q^2 p$$
$$-ip_t = -p_{xx} - 2p^2 q$$

Semidiscretised version

$$i\dot{q}_n = -\frac{q_{n-1} + q_{n+1} - 2q_n}{(\Delta x)^2} - p_n q_n (q_{n-1} + q_{n+1})$$
$$-i\dot{p}_n = -\frac{p_{n-1} + p_{n+1} - 2p_n}{(\Delta x)^2} - p_n q_n (p_{n-1} + p_{n+1})$$

AL Truncation Cont'd

It has a noncanonical Hamiltonian form

$$\dot{z} = P(z)\nabla H(z), \; z = (p, q)$$

$$H = \frac{i}{(\Delta x)^3}\sum_n (\Delta x)^2 p_n (q_{n-1} + q_{n+1}) -$$

$$2\ln(1 + (\Delta x)^2 q_n p_n)$$

$$P(z) = \begin{pmatrix} 0 & -R \\ R & 0 \end{pmatrix}$$

$$R = \operatorname{diag}\left\{\frac{1 + (\Delta x)^2 q_n p_n}{\Delta x}\right\}_{n=1}^{N}$$

Conclusions—Structure Preserving Integrators

- The literature (Islas et al.) report excellent long time behaviour of the presented approaches.
- Which approach is best depends on the parameters of the problems and the properties of interest.
- It is admitted that these geometric integrators are more expensive than classical ones.