Time integration for DNS of transitional and turbulent flow:

Critical evaluation of an IMEX method

Tapan K. Sengupta, Swagata Bhaumik, M. Sriramakrishnan
&
V. K. Sathyanarayanan

High Performance Computing Laboratory
Department of Aerospace Engineering
I.I.T. Kanpur, INDIA

URL: http://spectral.iitk.ac.in

Introduction

• Traditionally, both explicit and implicit time integration methods are used for solving IBVP's.

• **Explicit methods** are further classified into:

(a) **Single-stage, multi-step methods** (e.g., **Leap-Frog**, **Adams-Bashforth**, **BDF2** methods etc.) – which suffer from spurious numerical modes. The spurious modes smoothen the solution and hence these methods are very popular. But, these are of little use for DNS or even LES.

(b) **Multi-stage, single step methods** (e.g., **explicit Runge-Kutta methods**) do not suffer above problem and is recommended. A drawback is the requirement of small time step due to **numerical instability**.

• **Implicit methods** do not suffer **numerical instability** and hence seems attractive.

Introduction

• **Combination of implicit and explicit methods** used in domain decomposition mode is known as **IMEX method** and apparently is gaining in popularity.

• This has been used in **Sayadi, Hamman & Moin (JFM, 2013), Kanevsky et al. (JCP, 2007). Ascher et al. (SINUM, 1995), Ruuth (JMB,1995), Giraldo et al. (SISC, 2013)** and in Ph.D. theses of **Sayadi (Stanford U., 2012), Nagarajan (Stanford U., 2004)** among many other references. Even some physical events, such as bypass transition, have been reported in literature (Wu & Moin, JFM 2009) obtained by **IMEX method.**

• As there are no systematic studies to evaluate **IMEX methods,** present work is an exhaustive analysis of the same.

Basics of Global Spectral Analysis (GSA)

• This is based on tools developed by the authors and details are as in: **High Accuracy Computing Methods: Fluid Flows and Wave Phenomena. Cambridge Univ. Press, USA (2013)**

• One uses a **non-dissipative, non-dispersive model, 1D convection equation** to quantify numerical errors of any specific combination of spatial and temporal discretizations. This model equation for signal propagating to the right is,

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}; \qquad \text{for } c > 0$$

See use of this equation also in : i) **Lomax, Pulliam & Zingg (Springer, 2002)**; (ii) **Sengupta, Ganeriwal & De (JCP, 2003)**; (iii) **Sengupta & Dipankar (JSC, 2004); (iv) Sengupta et al. (JSC, 2006); (v) Trefethen (SISC, 1982); (vi) Haltiner & Williams (1958) and (vii) Vichnevetsky & Bowles (1981) etc.**

Basics of Global Spectral Analysis (GSA)

•GSA originally developed in **Sengupta et al. (JCP, 2003)** for full-domain following work of **Lele (JCP, 1992)** for spatial discretization alone.

• Space-time discretizations together was analyzed in **Haltiner & Williams (1958), Vichnevetsky & Bowles (1981)** and in **Sengupta & Dipankar (JSC, 2004), Sengupta et al. (JSC, 2006)** and "**High Accuracy Computing Methods: Fluid Flows and Wave Phenomena" – T K Sengupta, CUP (2013)**

• For **non-dissipative, non-dispersive 1D convection equation,** the numerical error was reported correctly for any spatial-temporal discretizations as

Basics of GSA (cont.)

$$\frac{\partial e}{\partial t}+c\frac{\partial e}{\partial x}=-c\left[1-\frac{c_N}{c}\right]\frac{\partial \overline{u}_N}{\partial x}-\int\frac{dc_N}{dk}\left[\int ik' A_0[|G|]^{t/\Delta t}e^{ik'(x-c_N t)}dk'\right]dk$$

$$-\int\frac{Ln|G|}{\Delta t}A_0[|G|]^{t/\Delta t}e^{ik(x-c_N t)}dk \qquad (1)$$

This is due to the correct numerical dispersion relation used:

$$\omega_{eq}=k\,c_N \qquad (2)$$

Where k is the wave number; c_N is the numerical phase speed and V_{gN} is the numerical group velocity, $d\omega_{eq}/dk$. G is the numerical amplification factor $U(k,t+\Delta t)/U(k,t)$.

This is to be contrasted with the traditional wrong numerical dispersion relation used:

$$\omega_{eq}=k_{eq}\,c \qquad (3)$$

Eqn. (1) is a consequence of Eqn. (2) – and not of Eqn. (3)!

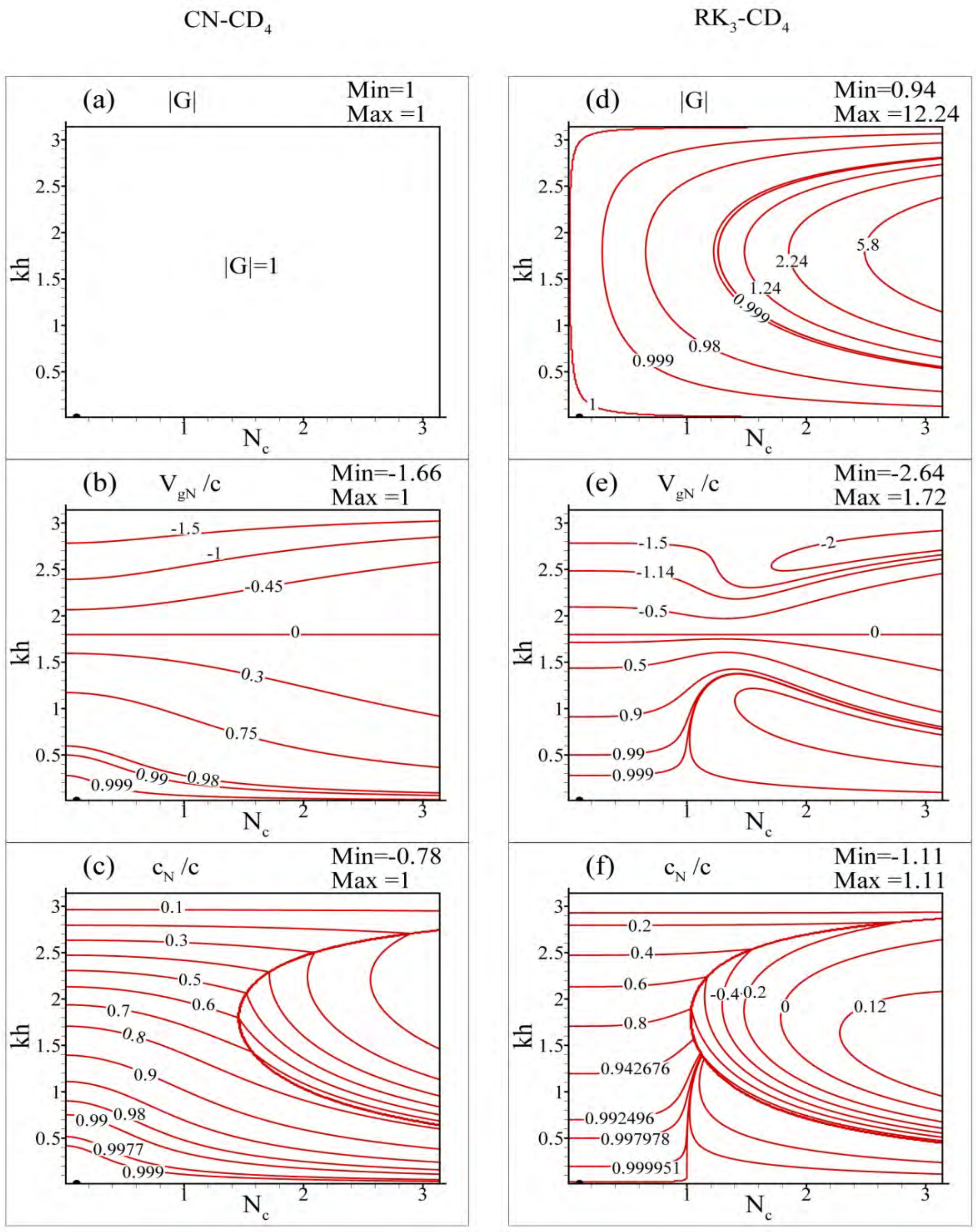
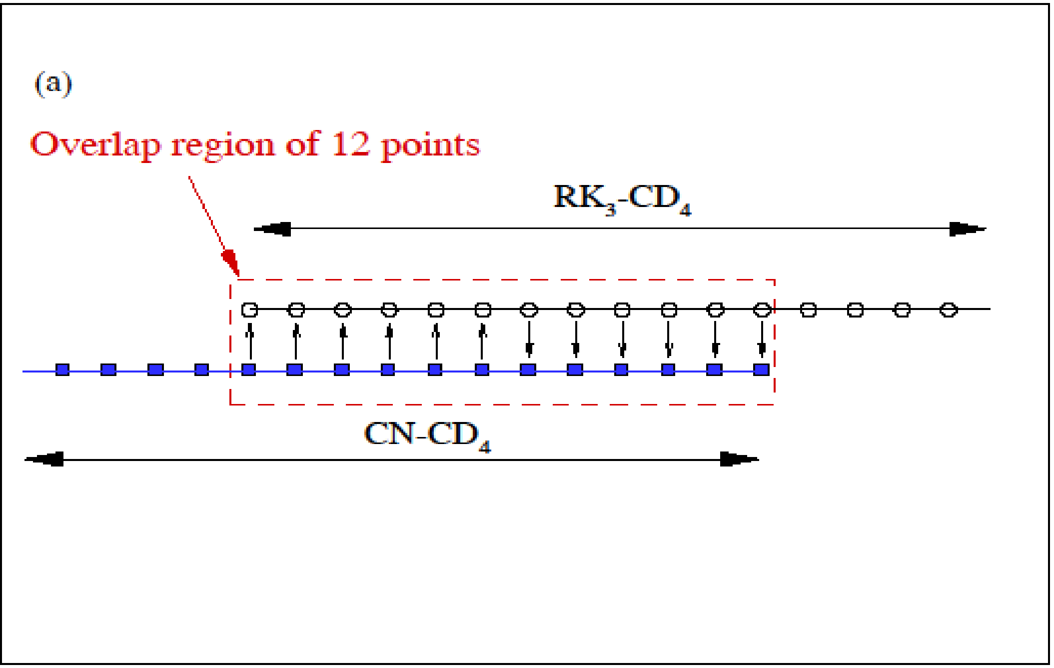
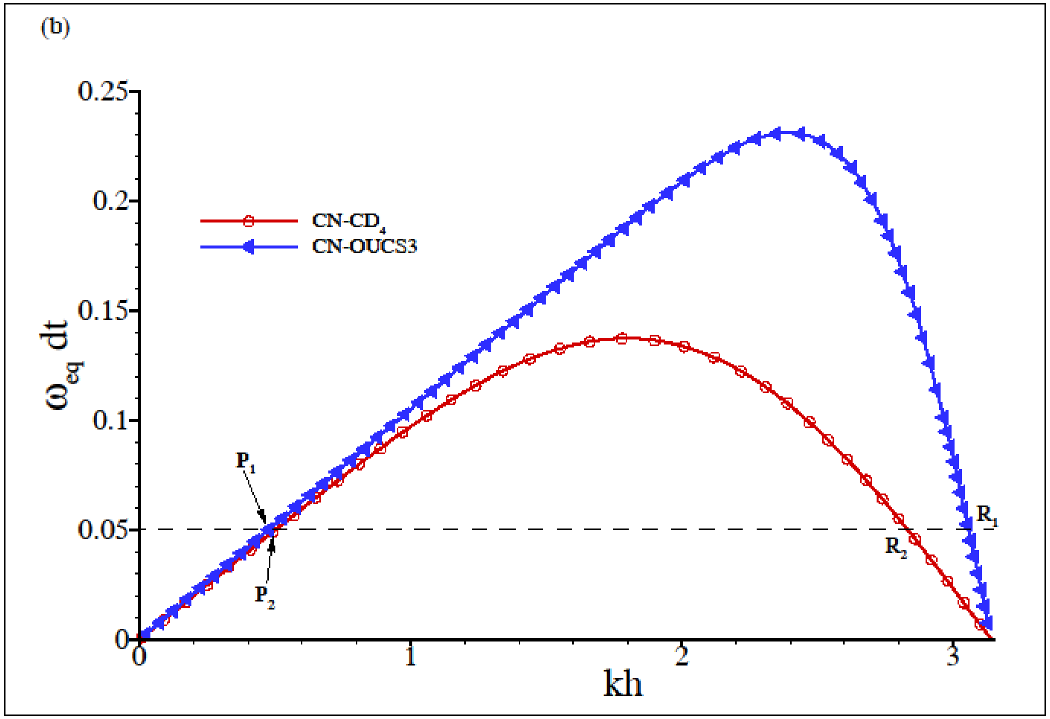


Fig. 1: Numerical properties of Implicit (Crank-Nicolson) and explicit (RK3) time integration methods used with CD4 spatial discretization for 1D convection equation.





IMEX METHOD
Preliminaries

Fig. 2(a) Schematic of overlap region with arrowheads showing data transfer for time integration. **(b)** Numerical dispersion relation for (CN-CD_4) and (CN-OUCS3) methods used to explain internal reflection at sub-domain boundaries.

Error Evolution using CD4 and OUCS3 Compact Schemes

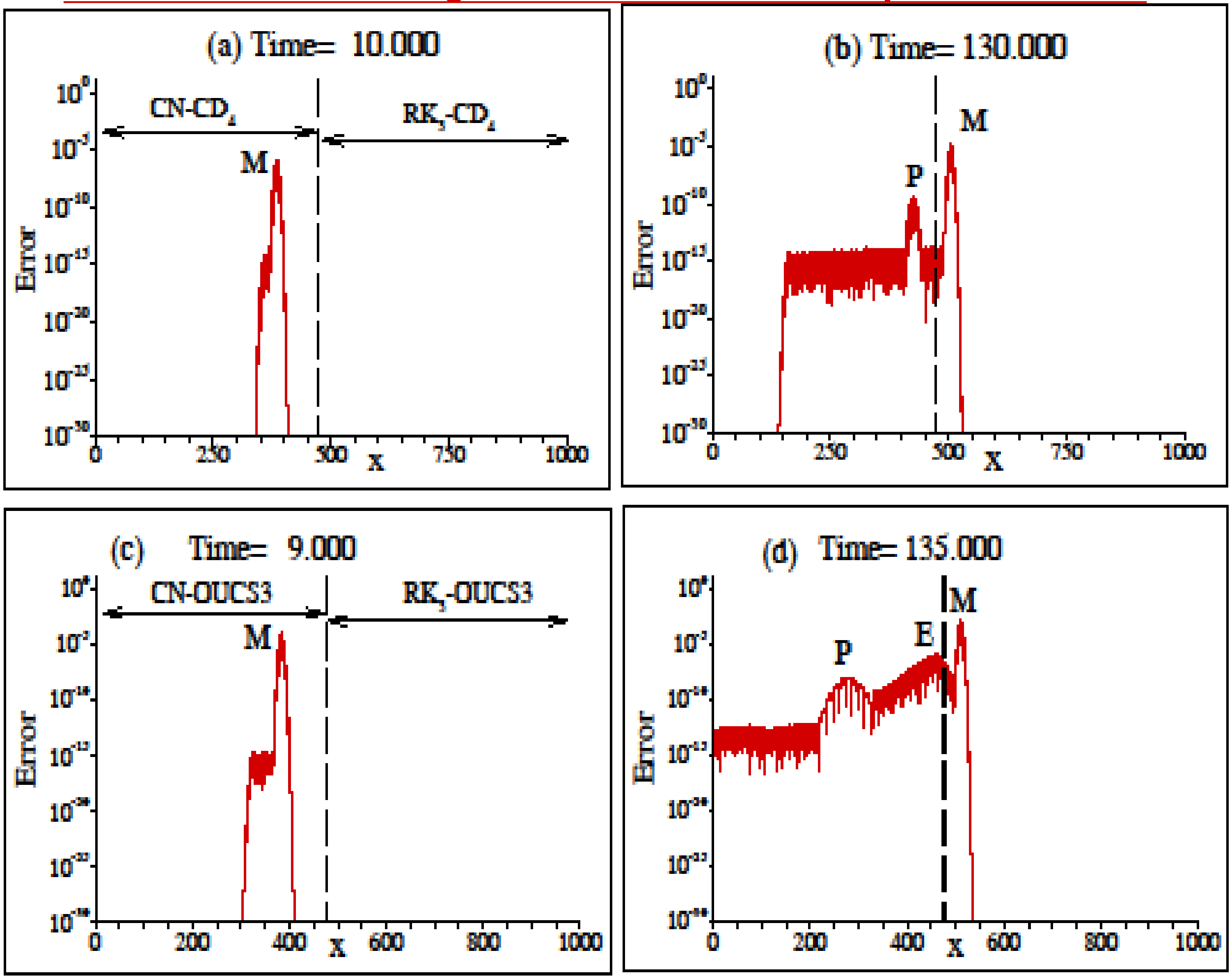


Fig. 3: Cases of 50 points overlap for solving 1D convection equation by IMEX method (a-b) using CD_4 scheme and (c-d) using OUCS3 scheme.

Solution of 1D convection equation by IMEX method with CD4 spatial discretization

- In Fig. 3(a-b), the peak M corresponds to error within the wave-packet that moves to the right which is of the order of 10^{-5}.
- When it crosses the overlap region, another spurious wave-packet (P) forms, which moves upstream and is of the order of 10^{-8}. This can be explained by Fig. 2.
- Here in the implicit part time integration is performed by using penta-diagonal solver.

Solution of 1D convection equation by IMEX method with OUCS3 spatial discretization

- Here in the implicit part, time integration is performed by using Bi-CGST**AB** iterative solver with tolerance of 10^{-9}.

- In Fig. 3(c-d), the peak M corresponds to error within the wave-packet that moves to the right which is of the order of 10^{-5}.

- When it crosses the overlap region, another spurious wave-packet (P) forms, which moves upstream and is of the order of 10^{-8}. This can be explained by Fig. 2.

- In between M and P, another peak at E is noted for OUCS3 scheme. This was absent for CD4 scheme, where accurate direct penta-diagonal solver is used for implicit part. This is explained next.

Solution of 1D convection eqn. by CD4 spatial discretization using indicated solvers

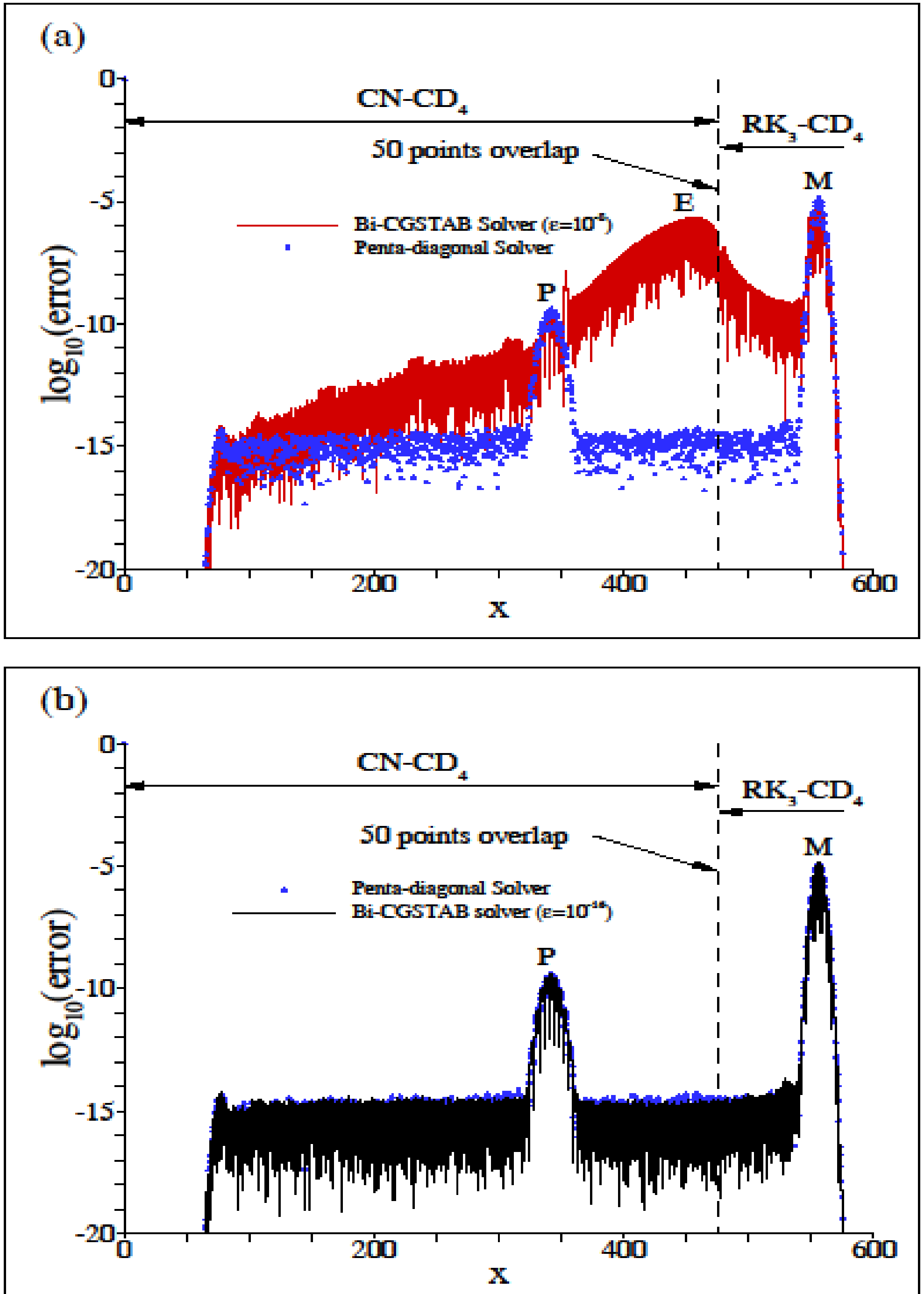


Fig. 4: (a) Comparison of error caused by direct penta-diagonal solver and Bi-CGSTAB iterative solver with the tolerance, ε =10^{-8}.

(b) Comparison of error caused by direct method and Bi-CGSTAB iterative solver with a tolerance, ε =10^{-16}.

Note: Using IMEX methods, one has to use iterative solver. When the peak M passes through the overlap region, the number of iterations doubles for ε = 10^{-16} as compared to that for ε =10^{-08}.

Two-Dimensional Linear Convection Equation

The model 2D linear convection equation which is used for more realistic and closer to Navier-Stokes equation. This is given as,

$$\frac{\partial u}{\partial t} + c_x \frac{\partial u}{\partial x} + c_y \frac{\partial u}{\partial y} = 0 \qquad (2.1)$$

where $c_x = c\cos\theta; c_y = c\sin\theta$ with θ as the angle of propagation. This Is solved with the initial condition

$$u = e^{-\alpha\left((x-x_0)^2+(y-y_0)^2\right)} \sin\left[k_0\sqrt{(x-x_0)^2+(y-y_0)^2} \right]$$

Here α *and* k_0 are parameters deciding the bandwidth of the wave-packet.

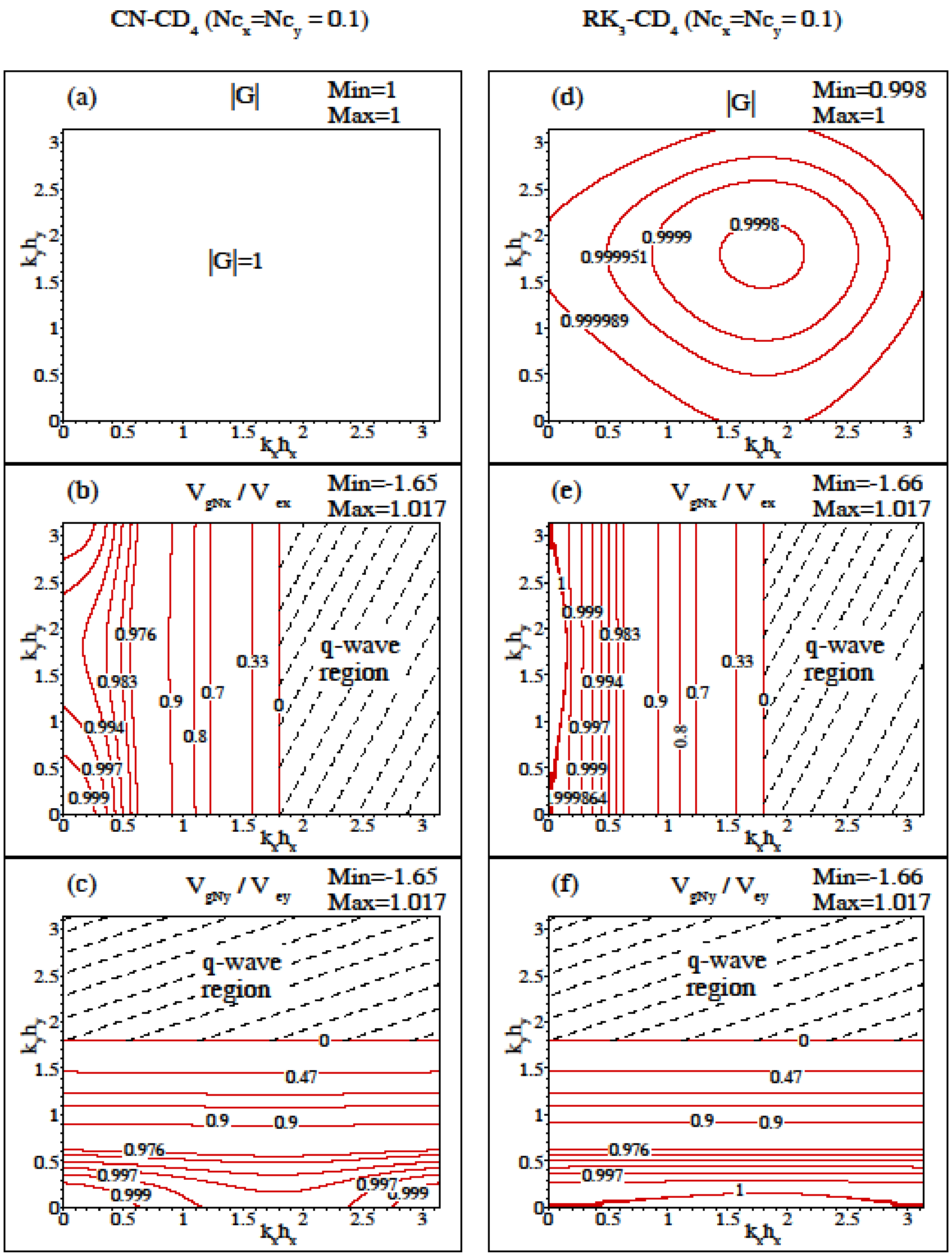


Fig. 5: Numerical properties of (CN-CD$_4$) and (RK$_3$-CD$_4$) schemes for solving Eqn. (2.1) : **(a) and (d)** Numerical amplification factor; **(b) and (e)** normalized numerical group velocity in x-direction and **(c) and (f)** normalized numerical group velocity in y-direction.

Note: Presence of q-wave region indicates spurious upstream propagating waves in solving the 2D convection problem.

Reference: Analysis of anisotropy of numerical wave solutions by high accuracy method- Sengupta et al., JCP, 230, 27-60 (2011)

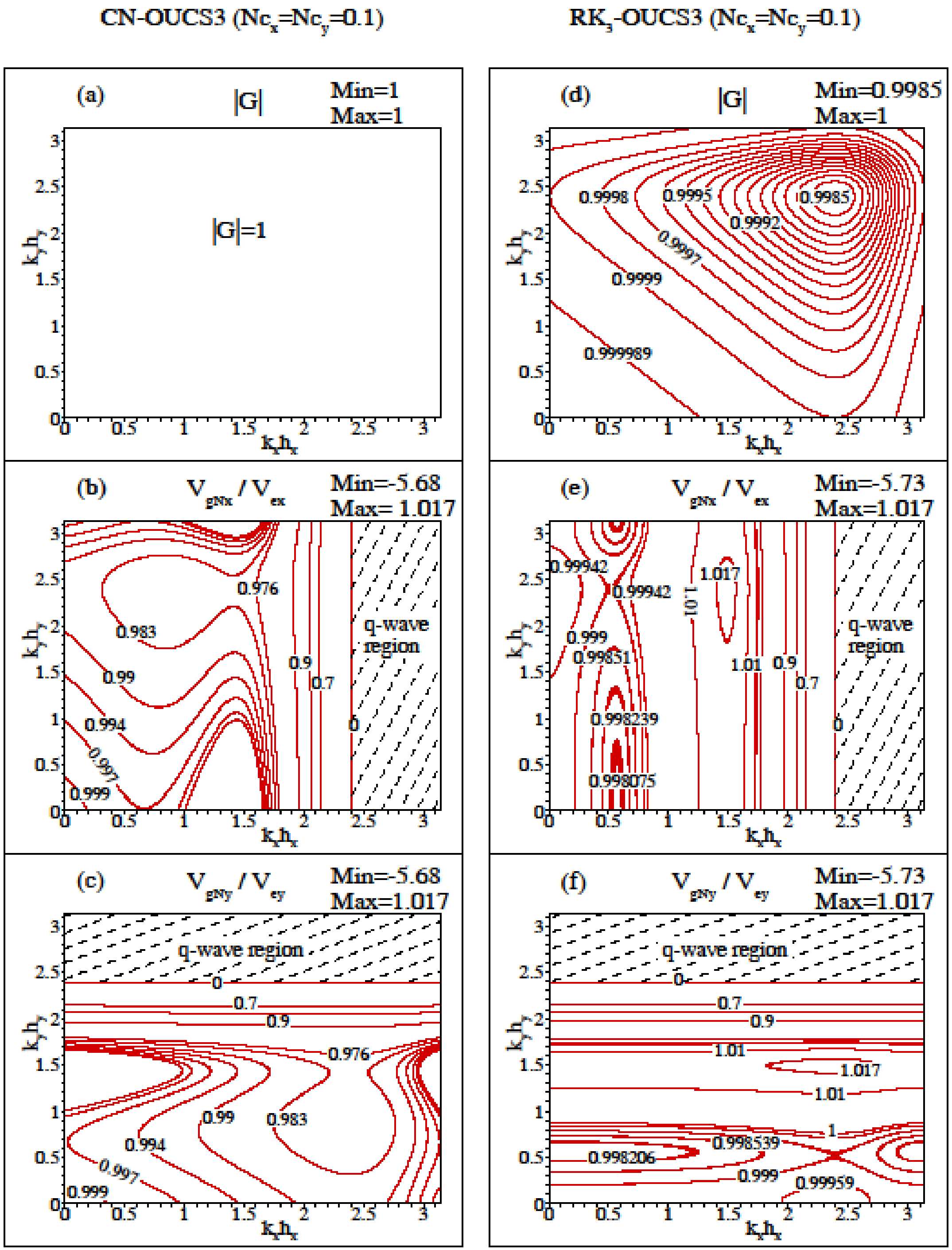


Fig. 6: Numerical properties of (CN-OUCS3) and (RK$_3$-OUCS3) schemes: **(a) and (d)** Numerical amplification factor; **(b) and (e)** normalized numerical group velocity in x-direction and **(c) and (f)** normalized numerical group velocity in y-direction.

Notes:

1) The q-wave region is significantly lower for compact scheme.

2) The range of values of |G| for compact scheme is almost near-neutral when used with RK3 method.

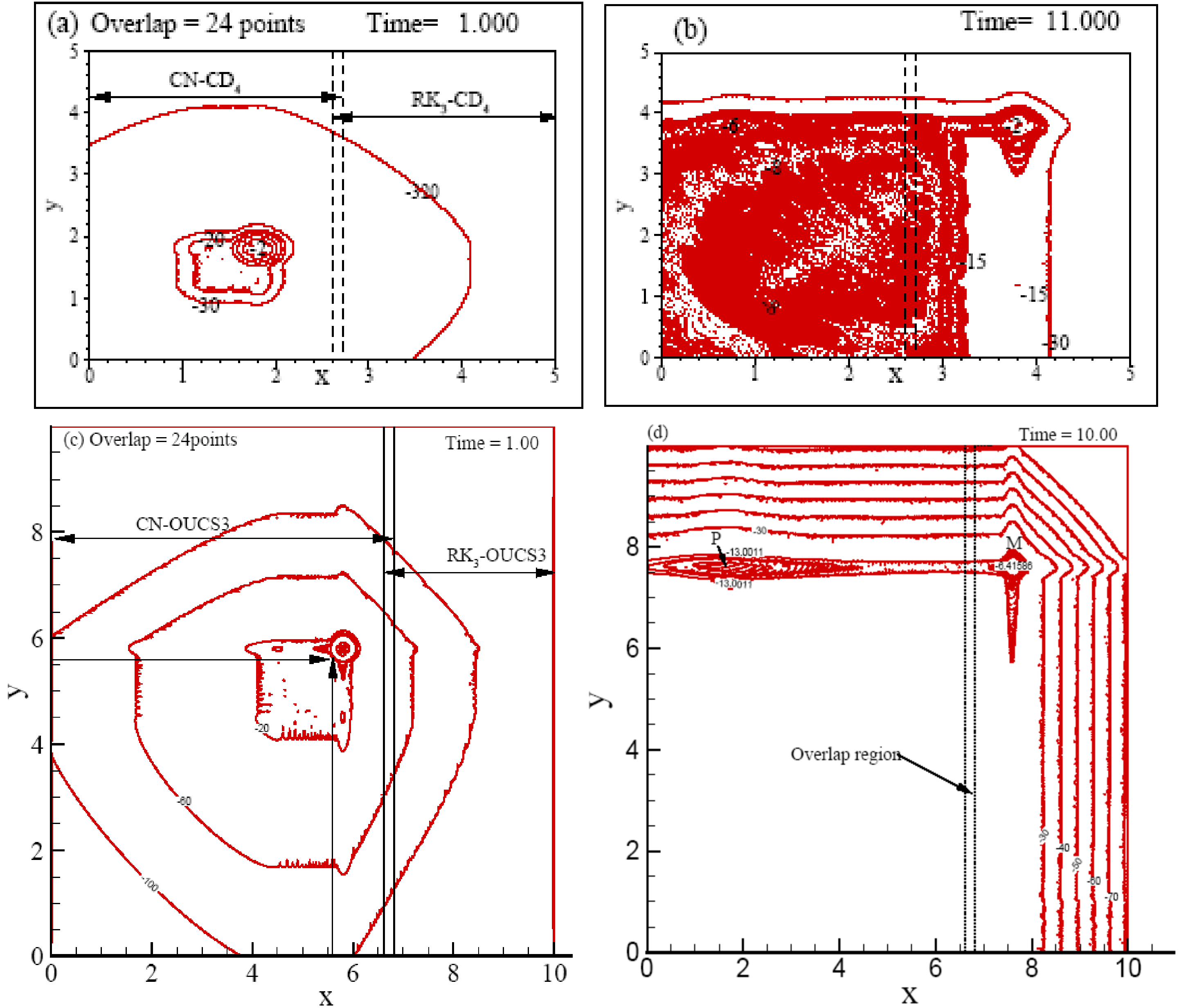


Fig. 7: Evolution of error for twenty four overlap points for the solution of 2D convection equation using CD_4 and OUCS3 spatial discretization in frames **(a)-(b) and (c)-(d),** respectively.

Results of 2D Convection Equation

- For the CD4 method, the main error packet has error is of the order 0.01, surrounded by lower error contours, as in frame (a).
- In frame (b), maximum error remains the same, but the upstream propagating error-packet reflects from the wall and approaches the domain-boundary which will create more packets. One can see 3 such packets in frame (b) for the CN-CD4 method. With time the number of packets will proliferate!
- For the OUCS3 method, the main error-packet is ten thousands times smaller as compared to CD4 method, as noted in frame (c).
- For the OUCS3 method in frame (d), the error-packet created by sub-domain boundary is orders of magnitude lower in strength.
- The error evolution for model equations will be shown at the end.

Role of IMEX Method for Three-Dimensional Flow Transition

• Next we solve Navier-Stokes equation for a shear layer excited by a Gaussian circular patch vibrated time harmonically (ω_o).

• Imposed wall-normal velocity created by the exciter is given by

$$v_{wall}(x,0,z,t) = \alpha_1 \, A_m(x,z) \, H(t) \; e^{i\omega_o t}$$

• Here, α_1 and $A_m(x,z) = \frac{1}{2}\left[1 + \cos\frac{\pi \, r}{r_{\max}}\right]$ define the amplitude of excitation.

•The exciter periodic in spanwise direction with a period of $z_{\max}$

• On a ZPG boundary layer, this creates planar and oblique 3D Tollmien-Schlichting wave-packets and not TS waves! All such theories of triad wave interactions are meaningless.

• Instead the creation and evolution of spatio-temporal wave-front is a more meaningful mechanism for transition ot turbulence. See Sengupta & Bhaumik (PRL, 2011) and Bhaumik & Sengupta (2014, PRE) for 2D and 3D transition. These require true DRP schemes, as discussed next.

3D Receptivity of Boundary Layer to Wall Excitation

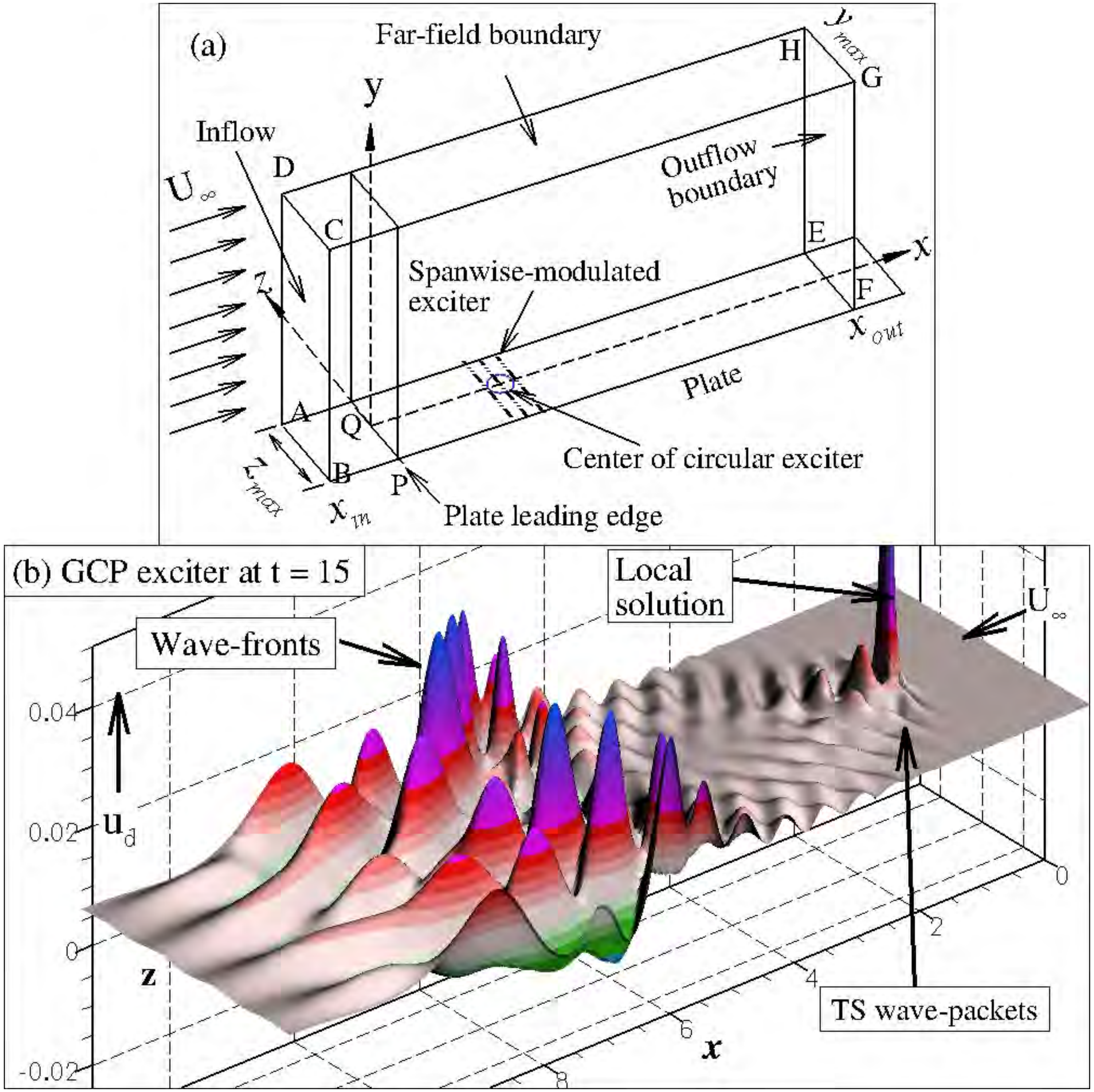
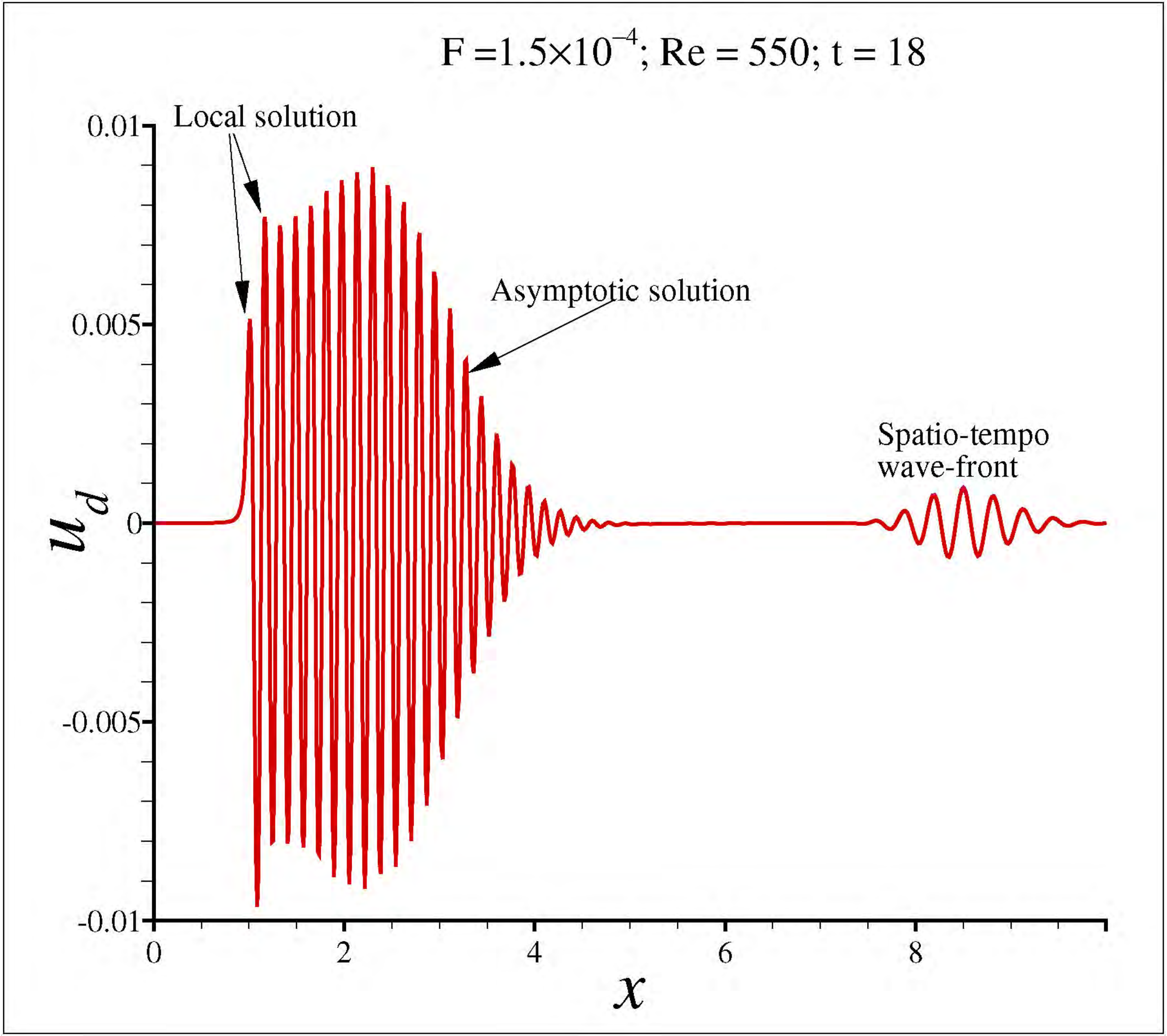
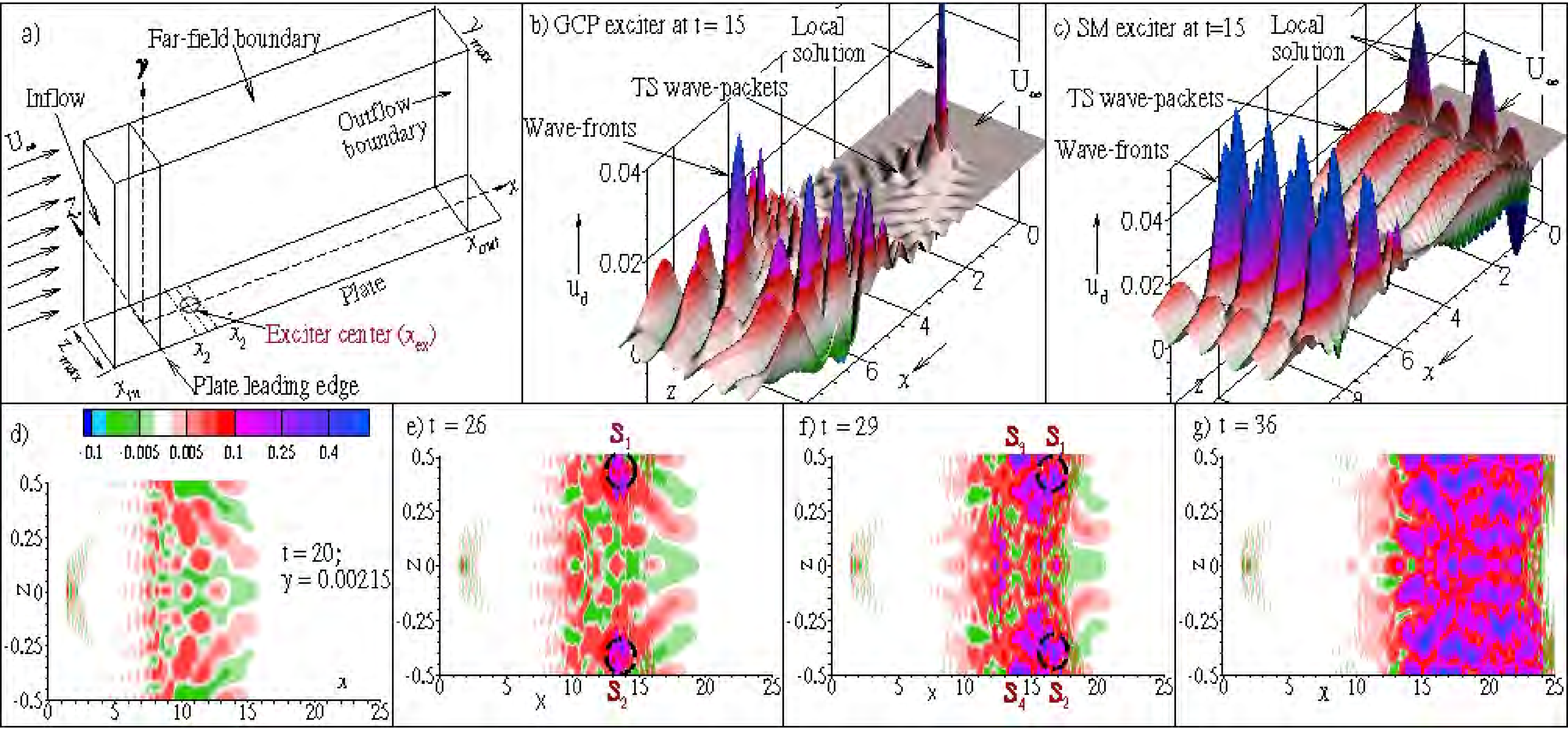


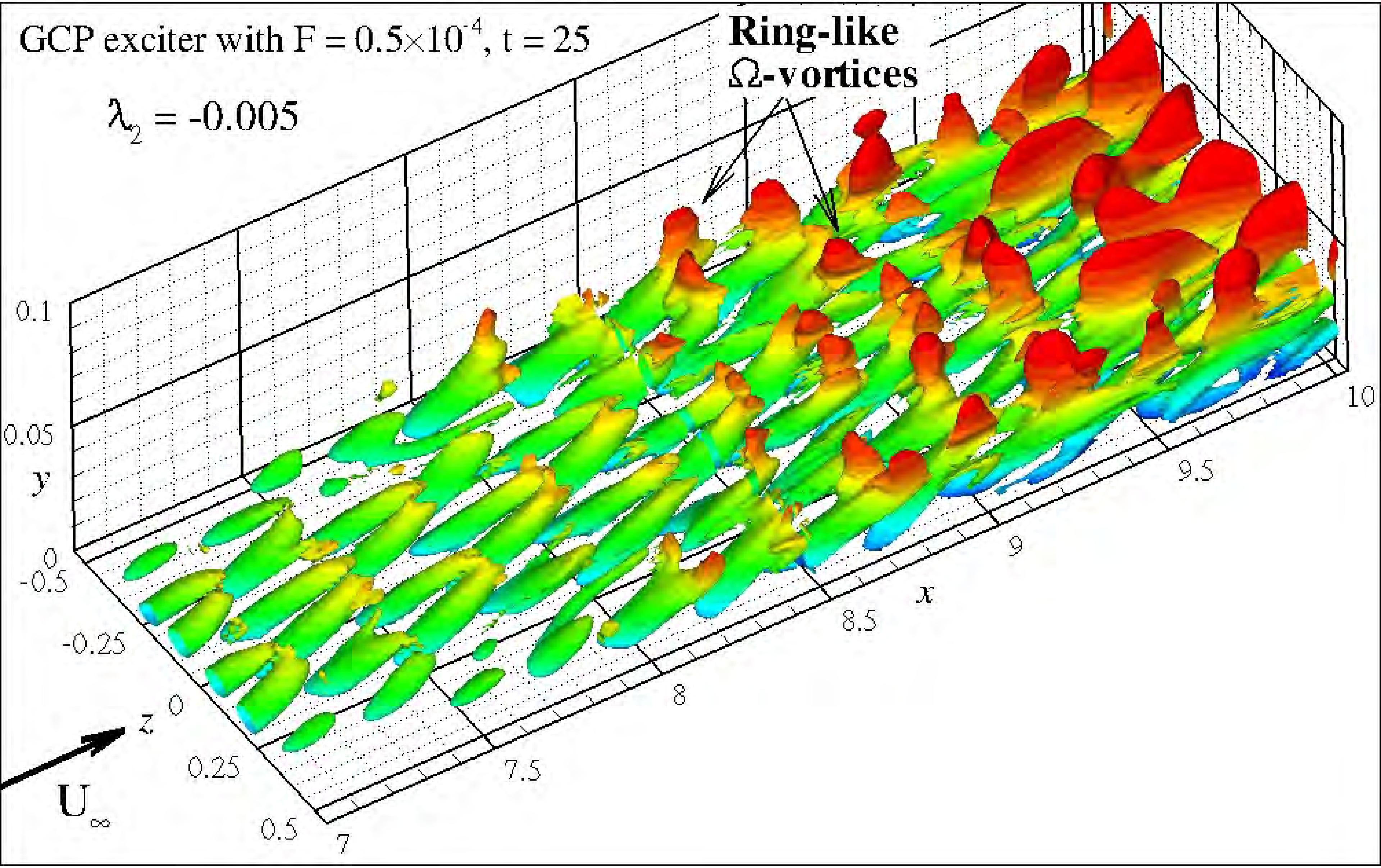
Fig. 8: **(a)** Schematic of the computational domain for Gaussian circular patch (GCP) exciter with center located at x_{ex} used in Bhaumik & Sengupta (PRE, 2014) **(b)** Perspective plot of streamwise disturbance velocity at a height y/L=0.00215 for t=15 after onset of GCP excitation, for a case with x_{ex} =1.5 and nondimensional frequency, F= 5 $\times 10^{-5}$ for 1% excitation amplitude and Reynolds number is Re = 10^5.



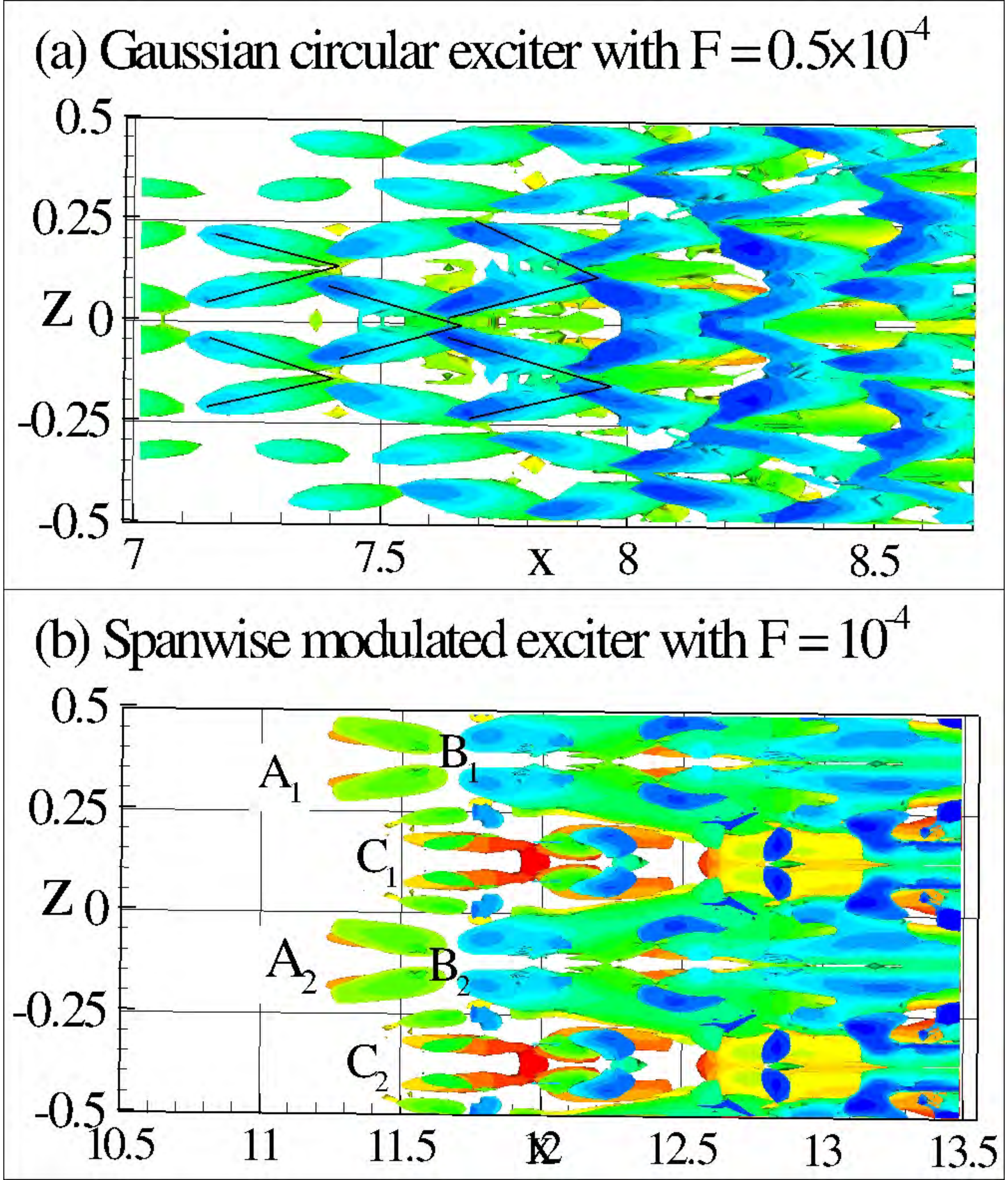
F =1.5×10^{-4}; Re = 550; t = 18
Local solution
Asymptotic solution
Spatio-tempo
wave-front
0.01
0.005
0
-0.005
-0.01
u_d
0
2
4
6
8
x



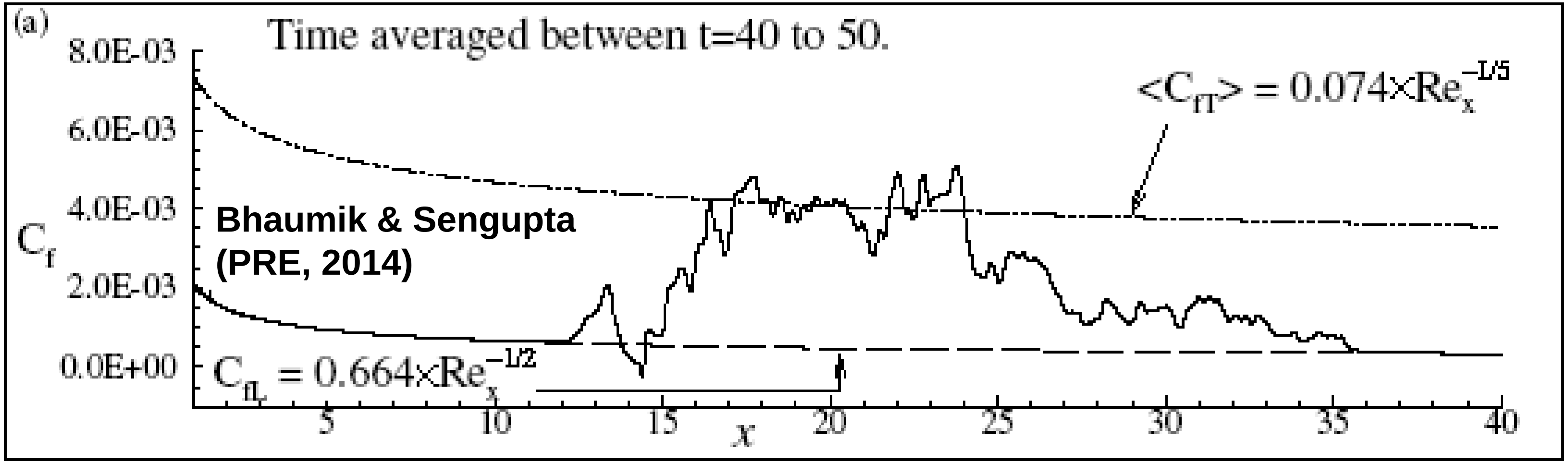
a)
Far-field boundary
Inflow
Outflow boundary
Plate
Exciter center (x_{ex})
Plate leading edge
b) GCP exciter at t = 15
Local solution
TS wave-packets
Wave-fronts
c) SM exciter at t=15
Local solution
TS wave-packets
Wave-fronts
d)
t = 20;
y = 0.00215
e) t = 26
f) t = 29
g) t = 36

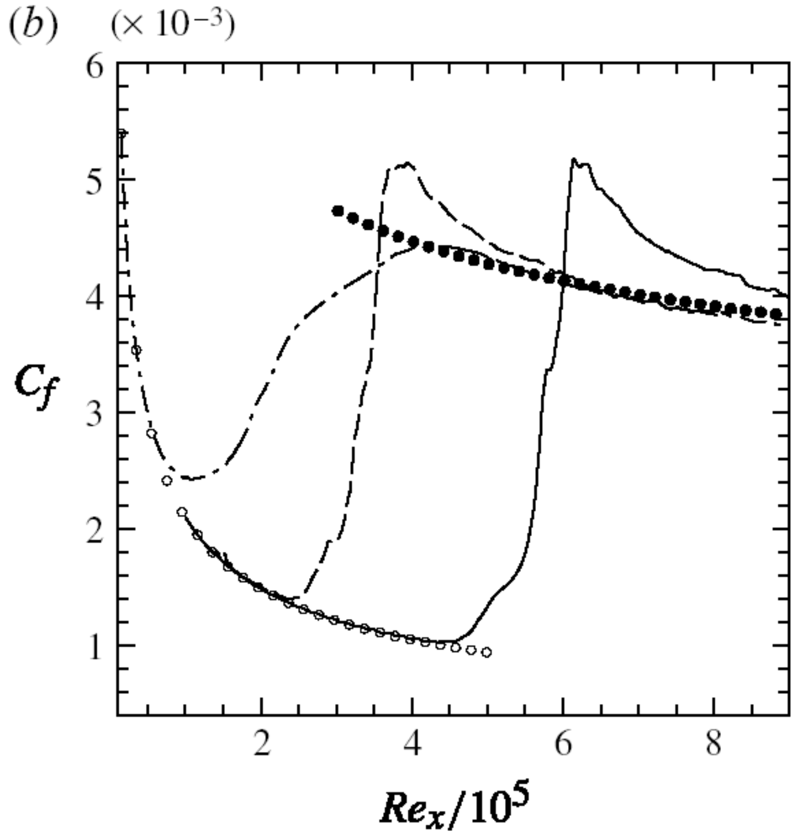


GCP exciter with F = 0.5×10^-4, t = 25
λ2 = -0.005
Ring-like
Ω-vortices
0.1
0.05
y
0
-0.5
-0.25
0
z
0.25
0.5
U∞
7
7.5
8
8.5
x
9
9.5
10



(a) Gaussian circular exciter with F = 0.5×10^-4
0.5
0.25
z 0
-0.25
-0.5
7
7.5
x
8
8.5
(b) Spanwise modulated exciter with F = 10^-4
0.5
0.25
z 0
-0.25
-0.5
A1
B1
C1
A2
B2
C2
10.5
11
11.5
12
x
12.5
13
13.5





Sayadi *et al.* (JFM, 2013) computed results with laminar and turbulent skin friction variation shown by discrete points.

Figure 8: Comparison of computed time-averaged wall skin friction by (a) the OCRK3 method in ***Bhaumik & Sengupta*** (PRE, 2014) and (b) the IMEX method in **Sayadi *et al.*** (JFM, 2013).

IMEX method versus explicit method of time integration of Navier-Stokes equation for DNS of transitional flows

- In Sayadi (Ph.D. thesis, Stanford U., 2012) and Sayadi *et al.* (JFM, 2013) IMEX method was used with a thin implicit layer very close to the flat plate. Although in the thesis, it is noted that the spatial discretization is by CD4 method, but in Sayadi *et al.* (2013), this is reported as staggered compact schemes for derivatives and filtering.

- In Fig. 7(a-b), we have noted that IMEX method for 1D convection equation produces q-waves and which proliferates after repeated reflections from domain boundaries and partial reflection/ refraction from boundary of implicit and explicit zone.

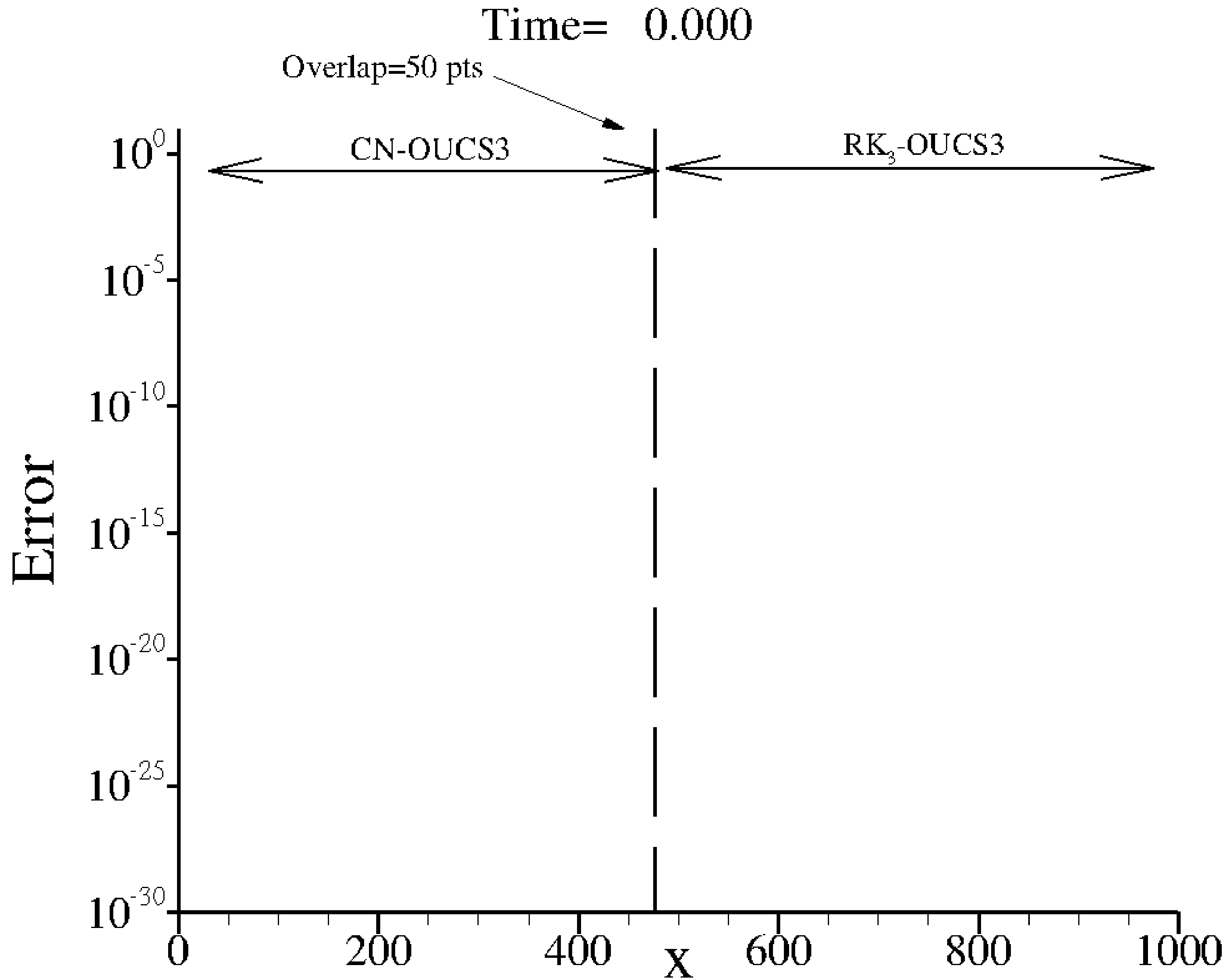
- In Sayadi *et al.* (JFM, 2013), the domain length was only 10, while in Bhaumik & Sengupta (PRE, 2014) this length was up to 50. The property of the used optimal staggered compact scheme is shown in Fig. 7(c-d), which shows only the partial reflection and refraction from sub-domain boundary and the error is four to five orders of magnitude lower.

IMEX method versus explicit method of time integration of Navier-Stokes equation for DNS of transitional flows

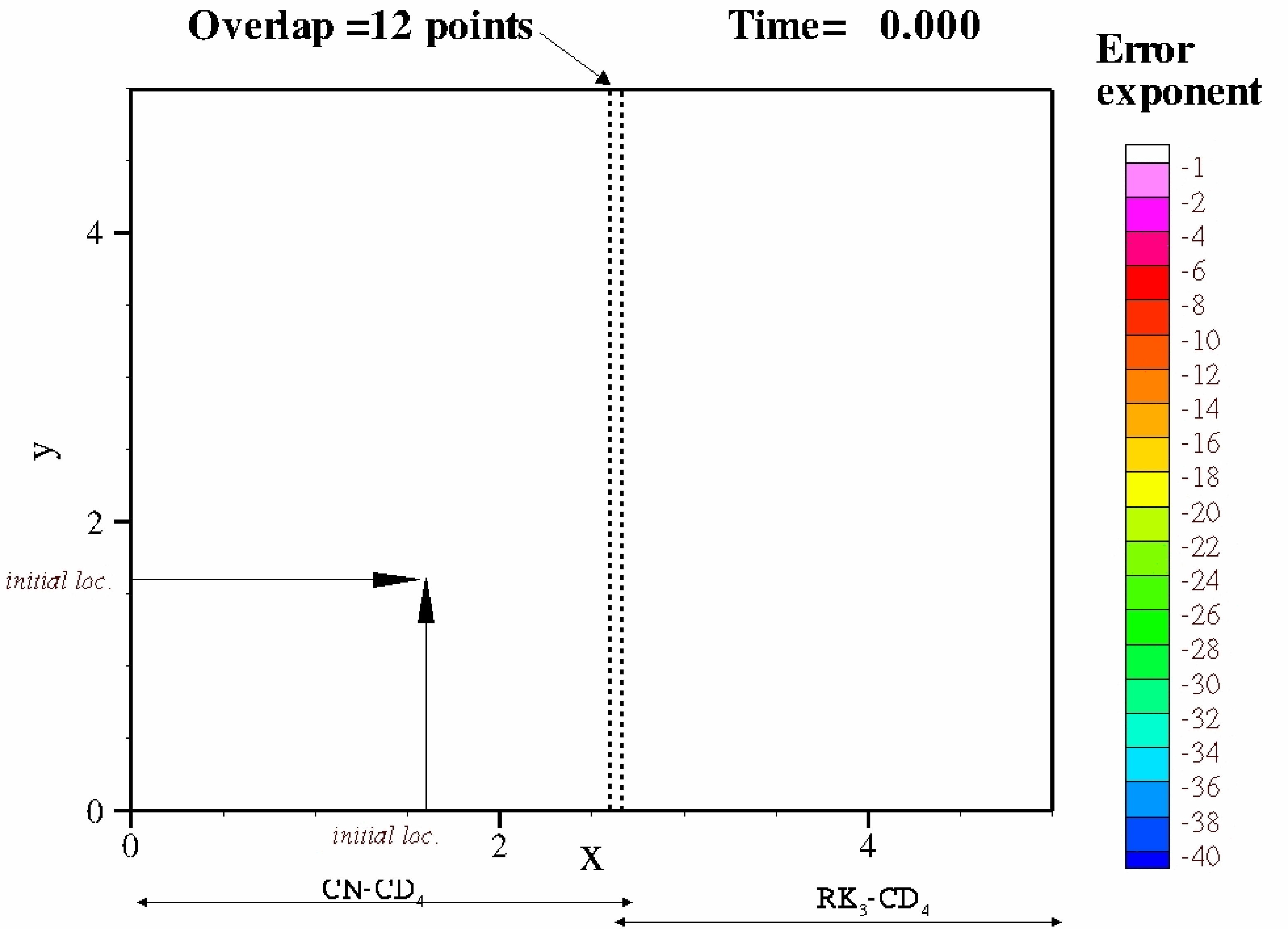
- In Sayadi *et al.* (JFM, 2013) no STWF was noted. The "computed transition" occurred in a short domain and transition from laminar to turbulent state was shown to be excellent!
- **This raises some fundamental questions:**

1. Can one obtain turbulent flows disregarding the physical process of transition?
2. Can any faulty numerical methods be used for DNS of transitional and turbulent flows?
3. In this scenario, one cannot distinguish between natural and bypass transition – a very troublesome feature! At the same time, it opens up avenues of systematic studies by correct methods.

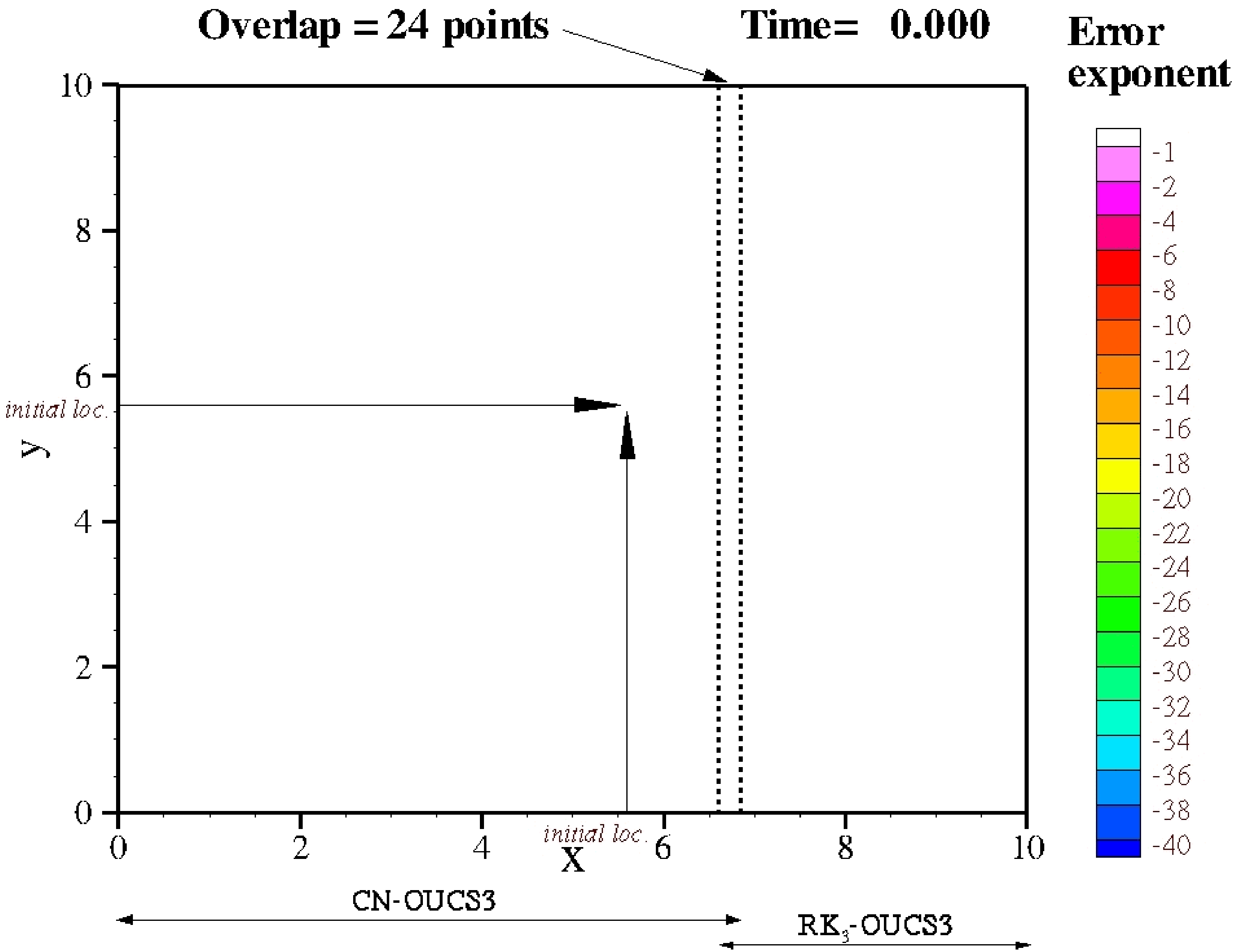
- For the sake of probity, it is important to reproduce the results of Sayadi (2012) and Sayadi *et al.* (2013), considering the fact that the actual method used in the work is not unambiguously reported.
- **Present results clearly shows that IMEX method is not correct for DNS.**



Error evolution in 1D wave propagation using IMEX time integration schemes along with OUCS3 spatial discretization



Error evolution in 2D wave propagation using IMEX time integration schemes along with CD_4 method of spatial discretization



Error evolution in 2D- wave propagation using IMEX (CN & RK_3) time integration schemes with OUCS3 for spatial discretization

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