

Case 3.5: Fourier Pseudo-Spectral Method

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Numerical Methods Overview

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 - ▶ Low order: Implicit midpoint rule (IMR) with a fixed time step solved by fixed point iteration.
 - ▶ High order: 4th-order explicit Runge-Kutta method developed by Carpenter-Kennedy with the Crank-Nicolson method for the viscous terms with fixed step.

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- ▶ Both time stepping schemes are done in Fourier space with the exception of the nonlinear terms that computed into real space.
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Implicit Midpoint Rule

$$\begin{aligned}
 & \frac{\mathbf{u}^{n+1,j+1} - \mathbf{u}^n}{\delta t} + \frac{\mathbf{u}^{n+1,j} + \mathbf{u}^n}{2} \cdot \nabla \left(\frac{\mathbf{u}^{n+1,j} + \mathbf{u}^n}{2} \right) \\
 = & \frac{\nabla \left[\Delta^{-1} \left(\nabla \cdot \left[(\mathbf{u}^{n+1,j} + \mathbf{u}^n) \cdot \nabla (\mathbf{u}^{n+1,j} + \mathbf{u}^n) \right] \right) \right]}{4} \\
 & + \Delta \frac{\mathbf{u}^{n+1,j+1} + \mathbf{u}^n}{2\text{Re}},
 \end{aligned}$$

Where u^n is the numerical solution at timestep t^n , and δt is the timestep size, and superscript j indicates the fixed point iterate.

Carpenter-Kennedy

Navier-Stokes divided into a linear,

$$l(u) = \frac{1}{\text{Re}} \Delta u \quad (1)$$

and nonlinear part

$$\mathbf{g}(\mathbf{u}) = -\mathbf{u} \cdot \nabla \mathbf{u} + \nabla [\Delta^{-1} (\nabla \cdot [\mathbf{u} \cdot \nabla \mathbf{u}])]. \quad (2)$$

Time stepping scheme is then,

$$\frac{d\mathbf{u}}{dt} = \mathbf{g}(\mathbf{u}) + l(\mathbf{u}) \quad (3)$$

Carpenter-Kennedy Algorithm

```
1: procedure RUNGE KUTTA(u)
2:   h = 0
3:   u = un
4:   for k = 1 → 5 do
5:     h ← g(u) +  $\beta_k$ h
6:      $\mu = 0.5\delta t(\alpha_{k+1} - \alpha_k)$ 
7:     v =  $\mu$ l(v) = u +  $\gamma_k\delta t$ h +  $\mu$ l(u)
8:     u ← v
9:   end for
10:  un+1 = u
11: end procedure
```

β , α , and γ are vectors of length 5 containing constants. Two levels of storage h and u .

Performance

- ▶ $\delta t = 0.005$ for 512^3 and $\delta t = 0.01$ for 256^3 grid points.
- ▶ For IMR scheme, fixed point iteration procedure was stopped once the difference between two successive iterates was less than 10^{-10} in l^∞ norm of velocity fields.

Method	Grid Size	Cores	Time Steps	Time(s)	$\frac{\text{Core Hours}}{\text{Time Step}}$
IMR	256^3	512	1000	4060	0.578
IMR	512^3	1024	500	9899	5.68
CK	512^3	4096	2000	7040	4.0

Table : Performance of Fourier pseudospectral code on Shaheen. IMR is an abbreviation for implicit midpoint rule and CK is an abbreviation for Carpenter–Kennedy.

Kinetic Energy Evolution

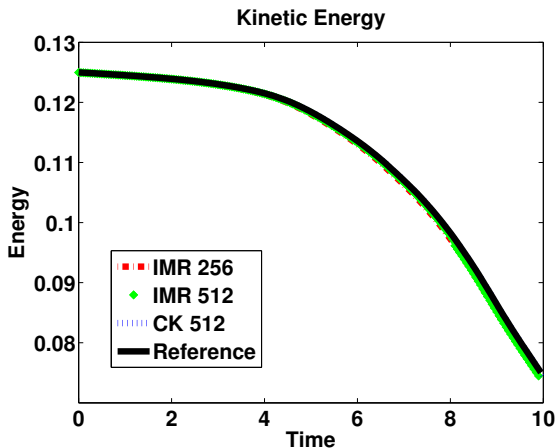


Figure : KE of solutions are so close they are almost indistinguishable

Kinetic Energy Dissipation Rate

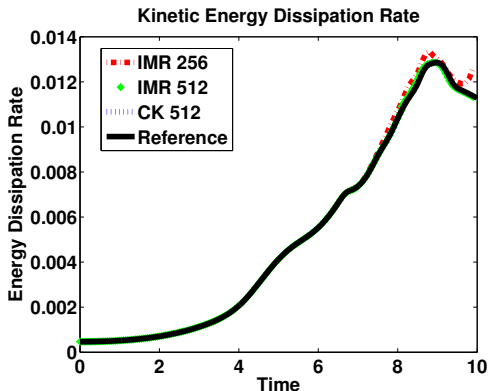


Figure : Plot during the initial stage, where flow is essentially inviscid and laminar. Fully developed turbulent flow is observed around $t_{max} \approx 8$.

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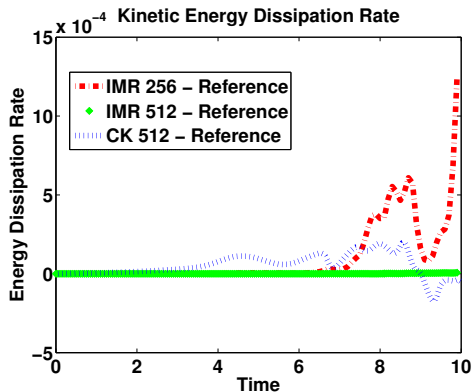


Figure : Difference in kinetic energy dissipation rates between the current discretizations and the reference solution.

Vorticity

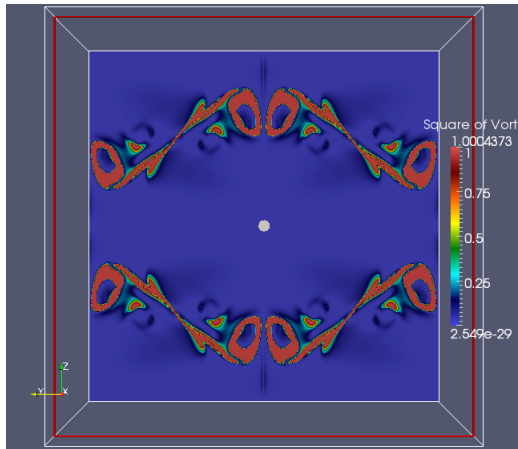


Figure : Square of the vorticity in the plane centered at $(\pi, 0, 0)$ with normal vector $(1, 0, 0)$.

Conclusion

- ▶ At almost the same computational cost, both 2nd-order accurate IMR and 4th-order Carpenter-Kennedy time stepping method, capture same amount of detail of the flow for 512^3 .
- ▶ Simulations with 256^3 grid points resulted in poor spatial convergences.