BS1 : Direct numerical simulation of the Taylor-Green Vortex at Re = 1600

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SPARK LES code basic topics

- Funded by Italian HYPROB Research program

  (finality: to develop capabilities and tools

  for design of Liquid Rocket Engines (LRE))

➢ Code solves fully compressible Navier-Stokes equations

➢ Taylor-Green vortex test-cases
  - Kinetic energy dissipation rate
  - Contours of vorticity norm
  - Kinetic energy power spectra

SPARK-LES code features at a glance

- Fortran 2008 standard
- Fully compressible, multi-species, reacting Navier-Stokes equations (cons. form)
- Finite-volume approach on curvilinear, structured multi-block grids
- Time accurate integration: up to fourth-order standard Runge-Kutta method
- High-order linear stencils for convective fluxes
  - ✓ Second and fourth-order explicit centered scheme (2E, 4E)
  - ✓ Fourth and sixth-order compact scheme (4C, 6C)
- Second order centered scheme for diffusive fluxes
- Jameson artificial dissipation up to fourth order and compact filters up to tenth order
- Real gas thermodynamics and Chemkin model
- Non-reflecting boundary conditions (NSCBC)
- Subgrid scale models (Smagorinsky, Wale)
- Full parallel capabilities (MPI paradigm)

Numerical schemes

- Finite volume: interpolate to interfaces cell-centered values
- General linear stencil

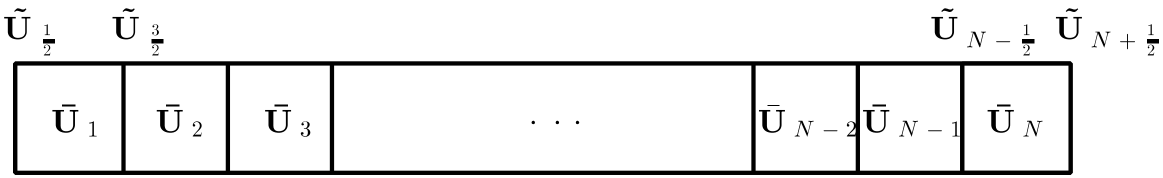
$$\alpha\tilde{\mathbf{U}}_{i-3/2}+\tilde{\mathbf{U}}_{i-1/2}+\alpha\tilde{\mathbf{U}}_{i+1/2}=\sum_{l=1}^{L}\gamma_l\left(\bar{\mathbf{U}}_{i-l}+\bar{\mathbf{U}}_{i+l-1}\right)$$

INTERFACES CELL CENTERS

- Explicit schemes (α=0)
  - Simple to implement and to parallelize
  - **Large stencils** and poor spectral resolution
- Compact schemes (α≠0)
  - Smaller stencil with respect to an explicit scheme at same order
  - Improved **resolution properties** (suitable for turbulent flows)
  - **Difficult to parallelize due to global domain dependence**

Statement of the problem

- Obtain interface values from cell-averaged values via a compact method
  - 1D, equally spaced domain
  - Tridiagonal, sixth-order compact scheme



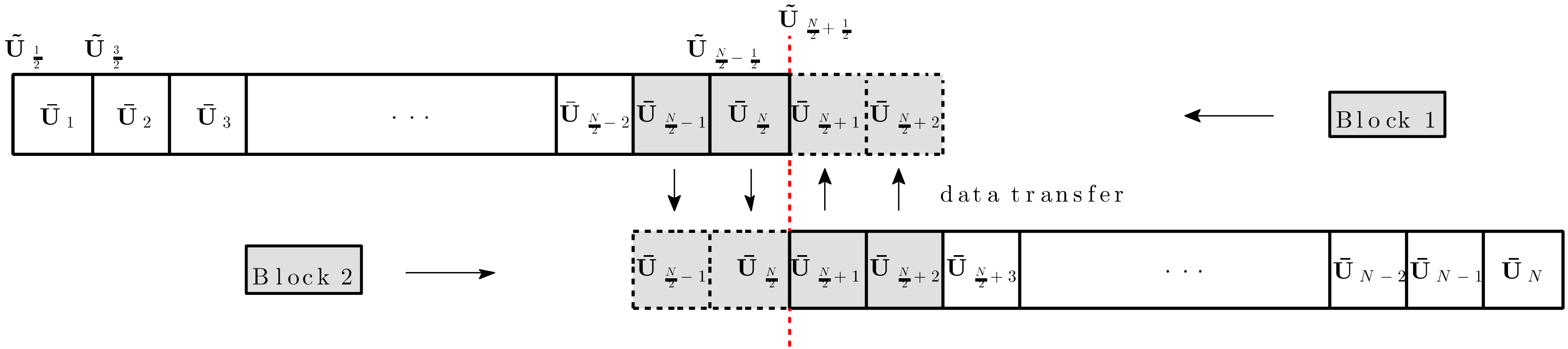
$$\alpha\tilde{\mathbf{U}}_{i-3/2} + \tilde{\mathbf{U}}_{i-1/2} + \alpha\tilde{\mathbf{U}}_{i+1/2} = \gamma_1\left(\bar{\mathbf{U}}_{i-1} + \bar{\mathbf{U}}_i\right) + \gamma_2\left(\bar{\mathbf{U}}_{i-2} + \bar{\mathbf{U}}_{i+1}\right)$$

$$\begin{bmatrix} \text{b.c.} & & & & & & & \\ & \ddots & & & & & & \\ & \alpha & 1 & \alpha & & & & \\ & & \alpha & 1 & \alpha & & & \\ & & & \alpha & 1 & \alpha & & \\ & & & & \alpha & 1 & \alpha & \\ & & & & & & \ddots & \\ & & & & & & & \text{b.c.} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{U}}_{1/2} \\ \vdots \\ \\ \\ \\ \\ \vdots \\ \tilde{\mathbf{U}}_{N+1/2} \end{bmatrix} = \begin{bmatrix} \text{b.c.} & & & & & & & \\ & \ddots & & & & & & \\ \gamma_2 & \gamma_1 & \gamma_1 & \gamma_2 & & & & \\ & \gamma_2 & \gamma_1 & \gamma_1 & \gamma_2 & & & \\ & & \gamma_2 & \gamma_1 & \gamma_1 & \gamma_2 & & \\ & & & \gamma_2 & \gamma_1 & \gamma_1 & \gamma_2 & \\ & & & & & \ddots & & \\ & & & & & & & \text{b.c.} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{U}}_1 \\ \vdots \\ \\ \\ \vdots \\ \bar{\mathbf{U}}_N \end{bmatrix}$$

Parallelization of compact schemes: possible approaches

- Algorithmic approaches: parallelization of linear system inversion
  - pipelined Thomas algorithm (PTA)
  - parallel diagonal dominant (PDD)
  - …
  - Drawbacks: **penalties in efficiency** and increased programming **complexity**
- Boundary Approximation Approach (BAA)
  - Used in domain decomposition techniques
  - Derivation of disjoint systems that can be solved independently
  - Drawbacks: **approximate solution** with respect to the serial one

Parallelization of compact (1)



$$\alpha\tilde{\mathbf{U}}_{i-3/2} + \tilde{\mathbf{U}}_{i-1/2} + \alpha\tilde{\mathbf{U}}_{i+1/2} = \gamma_1\left(\bar{\mathbf{U}}_{i-1} + \bar{\mathbf{U}}_{i}\right) + \gamma_2\left(\bar{\mathbf{U}}_{i-2} + \bar{\mathbf{U}}_{i+1}\right)$$

interior points (compact)

$$\tilde{\mathbf{U}}^{(1)}_{N/2+1/2} \equiv \tilde{\mathbf{U}}^{(2)}_{N/2+1/2} = b\left(\bar{\mathbf{U}}_{N/2-1} + \bar{\mathbf{U}}_{N/2+2}\right) + a\left(\bar{\mathbf{U}}_{N/2} + \bar{\mathbf{U}}_{N/2+1}\right)$$

shared interface (explicit)

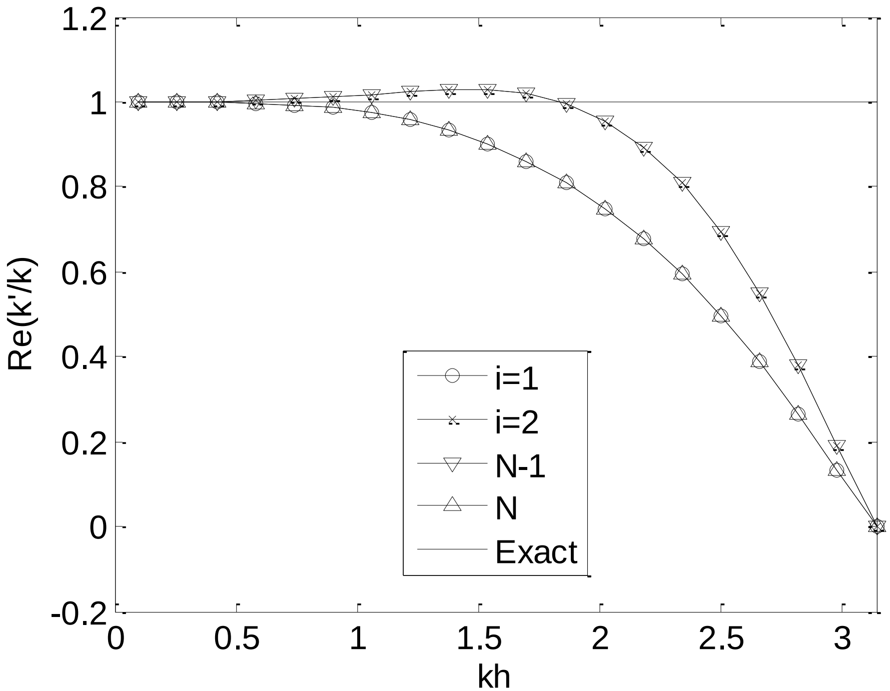
$$\begin{bmatrix} \text{b.c.} & & & & & & & \\ & \ddots & & & & & & \\ & \alpha & 1 & \alpha & & & & \\ & & \cancel{\alpha} & 1 & \cancel{\alpha} & & & \\ & & & \cancel{\alpha} & 1 & \cancel{\alpha} & & \\ & & & & \alpha & 1 & \alpha & \\ & & & & & & \ddots & \\ & & & & & & & \text{b.c.} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{U}}_{1/2} \\ \vdots \\ \tilde{\mathbf{U}}^{(1)}_{N/2+1/2} \\ \tilde{\mathbf{U}}^{(2)}_{N/2+1/2} \\ \vdots \\ \tilde{\mathbf{U}}_{N+1/2} \end{bmatrix} = \begin{bmatrix} \text{b.c.} & & & & & & & \\ & \ddots & & & & & & \\ \gamma_2 & \gamma_1 & \gamma_1 & \gamma_2 & & & & \\ & b & a & a & b & & & \\ & & b & a & a & b & & \\ & & & \gamma_2 & \gamma_1 & \gamma_1 & \gamma_2 & \\ & & & & & \ddots & & \\ & & & & & & & \text{b.c.} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{U}}_{1} \\ \vdots \\ \bar{\mathbf{U}}_{N/2-1} \\ \bar{\mathbf{U}}_{N/2} \\ \bar{\mathbf{U}}_{N/2+1} \\ \bar{\mathbf{U}}_{N/2+2} \\ \vdots \\ \bar{\mathbf{U}}_{N} \end{bmatrix}$$

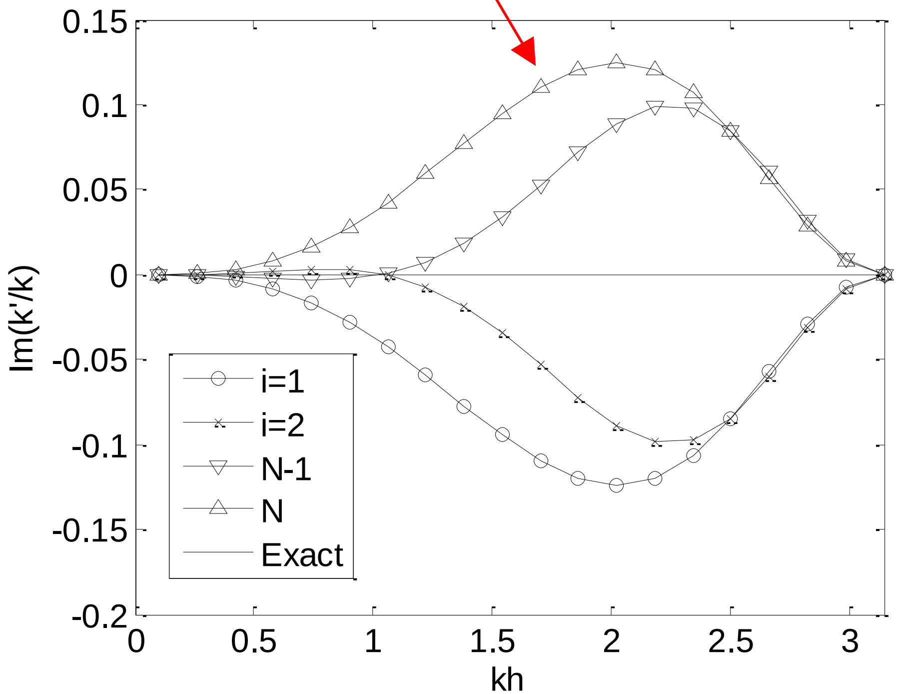
Parallelization of compact (2)

- Linear spectral resolution analysis on an equally spaced grid of step *h*
- Modification of the matrix coefficients leads to altered spectral properties

$$u(x) = e^{ikx}$$
$$u'_{\mathrm{ex}}(x) = iku(x)$$
$$\longrightarrow \quad \mathbf{u}' = i\mathbf{k}'\mathbf{u}$$

Anti-diffusion at mid-wavenumbers





Simulations matrix

- Three different resolutions (64, 128, 256 cubed) and four spatial schemes analyzed (12 cases)
- Regular cartesian meshes generated by an in-house Fortran code
- Third order explicit Runge-Kutta time advancement at CFL = 0.6
- No artificial dissipation or filters
- Computations run on 64 MPI cores over a CIRA cluster (CPU Intel Xeon E5-2680 @ 2.7 Ghz)
- Parallel compact: actually based on boundary approximation approach (BAA)

Parallel performances

- Parallel Speedup at different mesh resolutions and schemes

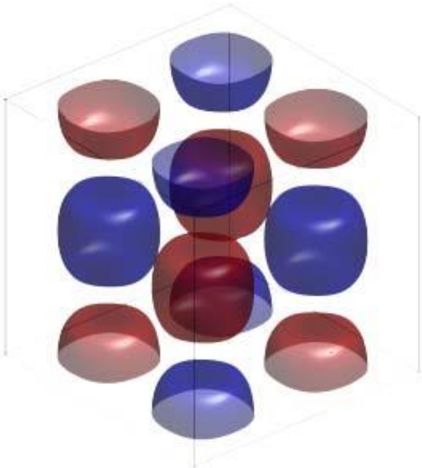
	2E	4E	4C	6C
64	51.091	42.456	37.077	36.274
128	46.216	41.067	37.763	37.262
256	50.049	44.180	40.995	40.732

- Structured grid leads to minor speedups
- At finest mesh resolutions speedups are generally good

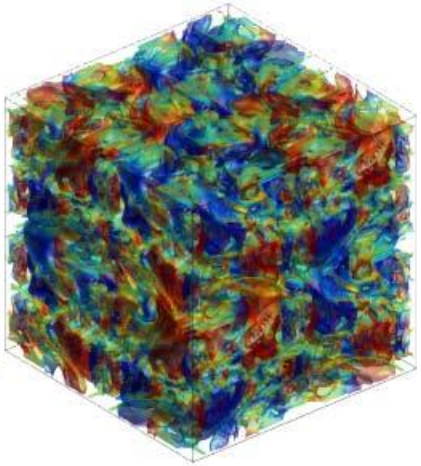
Taylor-Green Vortex (TGV)

- Prototype test for transition, dynamics of turbulence and decay
- Initial flow-field given by:

$$
\begin{cases}
u = \sin(x)\cos(y)\cos(z) \\
v = -\cos(x)\sin(y)\cos(z) \\
w = 0 \\
p = p_0 + \dfrac{\rho_0}{16}\left[\cos(2x)+\cos(2y)\right]\left[\cos(2z)+2\right]
\end{cases}
$$



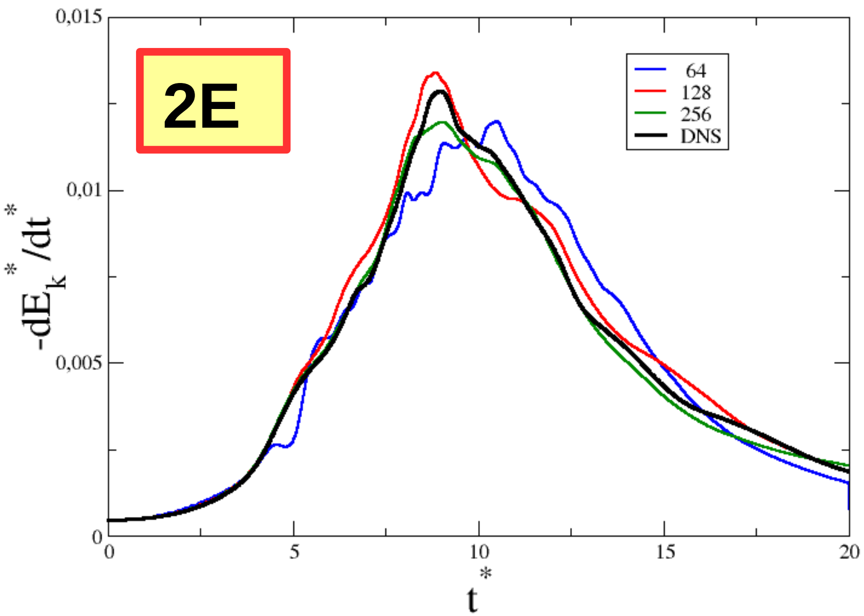
- 3D periodic box
- The flow undergoes creation of small scales due to vortex-stretching and initial distribution of vorticty
- Transition to turbulence occurs
- A turbulent decay phase follows due to action of viscosity and the absence of an external forcing

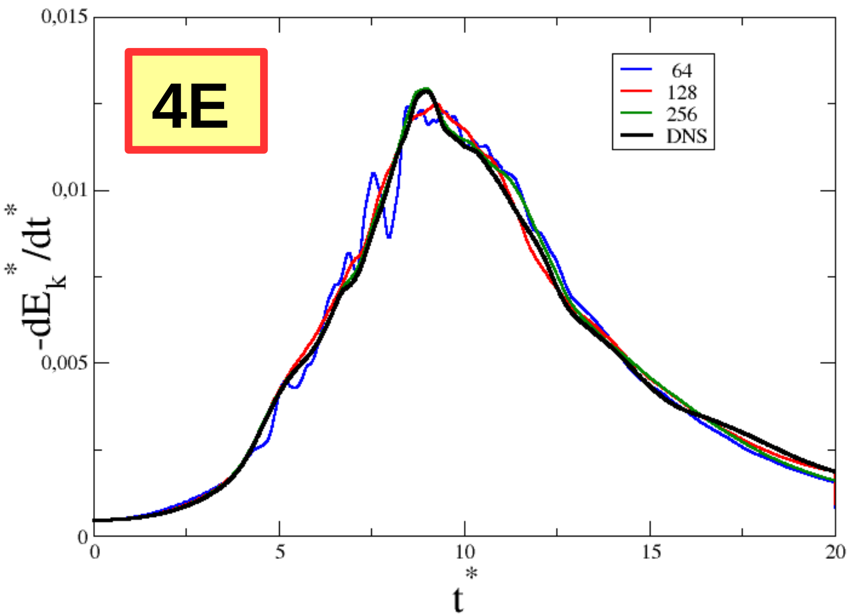


Kinetic energy decay rate : explicit schemes

Time-evolution of kinetic energy dissipation rate

$$-\frac{dE_k}{dt} = -\frac{1}{\rho_0 \Omega}\frac{d}{dt}\int_\Omega \rho \frac{\mathbf{u}\cdot\mathbf{u}}{2} d\Omega \approx 2\frac{\mu}{\rho_0 \Omega}\int_\Omega \mathbf{S}^d : \mathbf{S}^d d\Omega$$

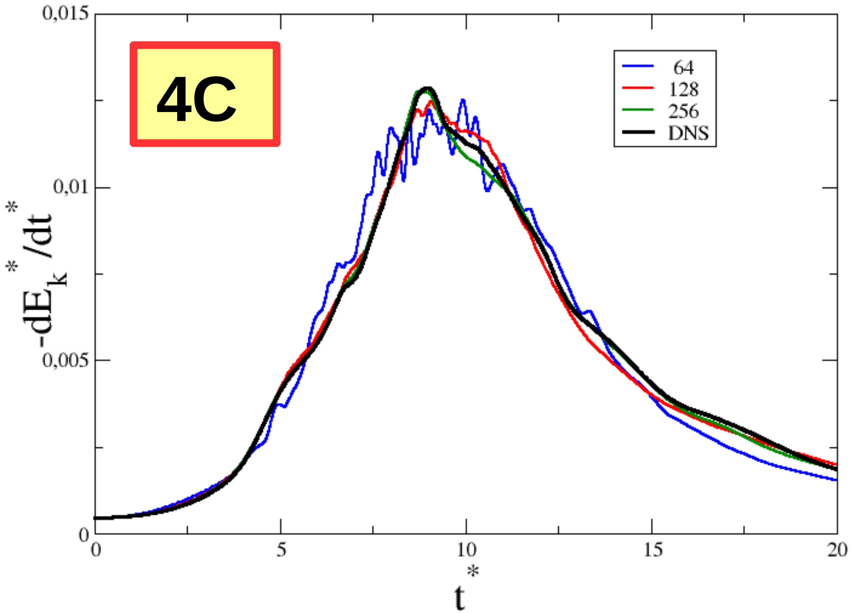


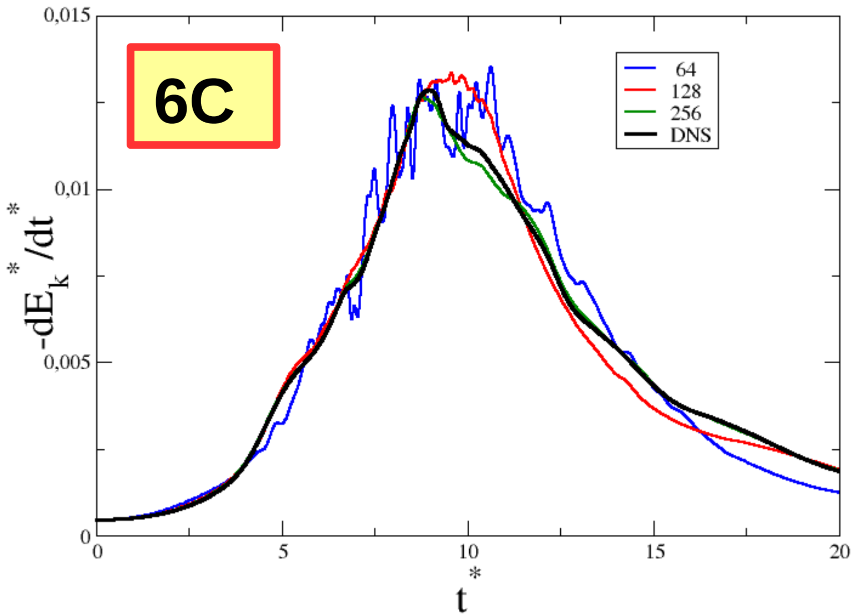


Kinetic energy decay rate : compact schemes

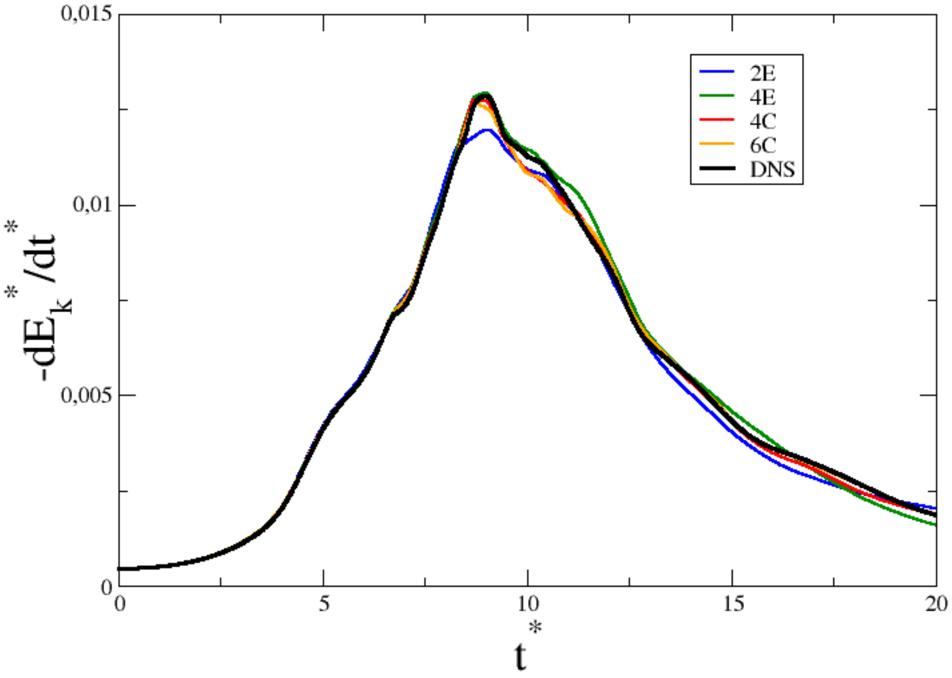
Time-evolution of kinetic energy dissipation rate

$$-\frac{dE_k}{dt} = -\frac{1}{\rho_0 \Omega}\frac{d}{dt}\int_\Omega \rho \frac{\mathbf{u}\cdot\mathbf{u}}{2} d\Omega \approx 2\frac{\mu}{\rho_0 \Omega}\int_\Omega \mathbf{S}^d : \mathbf{S}^d d\Omega$$





Kinetic energy decay rate : schemes comparison in 256^3 mesh



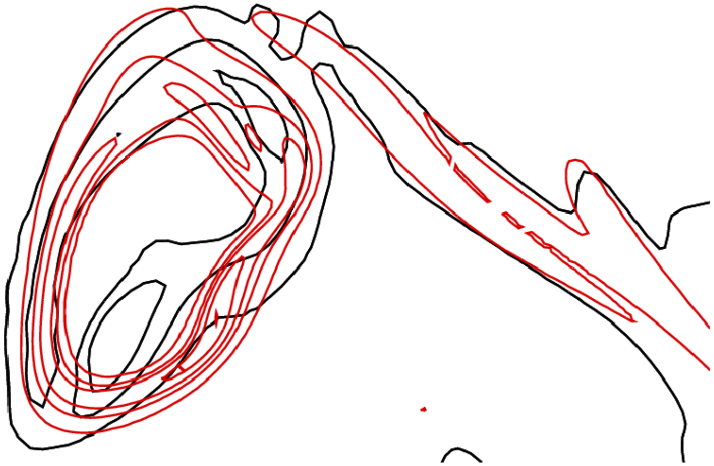
- transition to small scales (t*<7) : all schemes works properly
- massimum dissipation phase (t*~8) : 2E underestimate
- dissipation phase (t*>10) : good behavior of schemes

Contour of dimensionless vorticity norm: explicit schemes comparison, 256^3 mesh

2E

Red lines:
Reference solution

4E



Second order explicit scheme is not enough accurate

Contour of dimensionless vorticity norm: compact schemes comparison 256^3 mesh

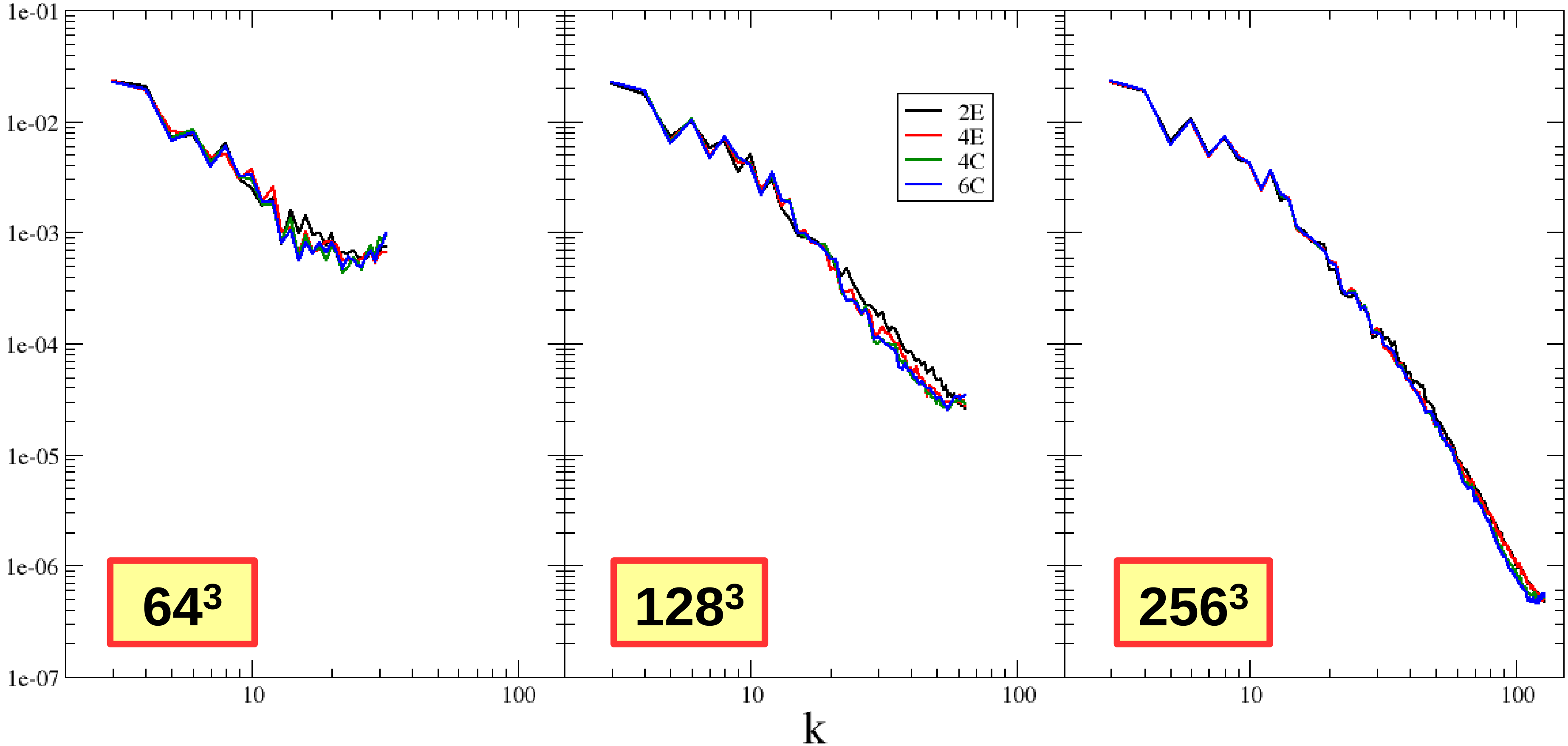
4C

Red lines:
Reference solution

6C

Satisfactory results

Kinetic energy power spectra at different mesh resolutions



- Energy spectra are substantially **independent** of the scheme
- Lowest resolutions show **energy pile-up at high wavenumbers**

Conclusions

- TGV test in order to assess code ability to describe turbulence over a wide range of energy scales
- On finest meshes results are **quite satisfactory** in the case of higher order schemes and a **good parallel efficiency is observed**
- Compacts schemes are promising, and better strategies in parallelization are currently under development

Thank you for your attention.

Any question, suggestion?