Low Order Methods for Simulation of Turbulence in Complex Geometries

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Petascale Computing:

Its Impact on Geophysical Modeling and Simulation

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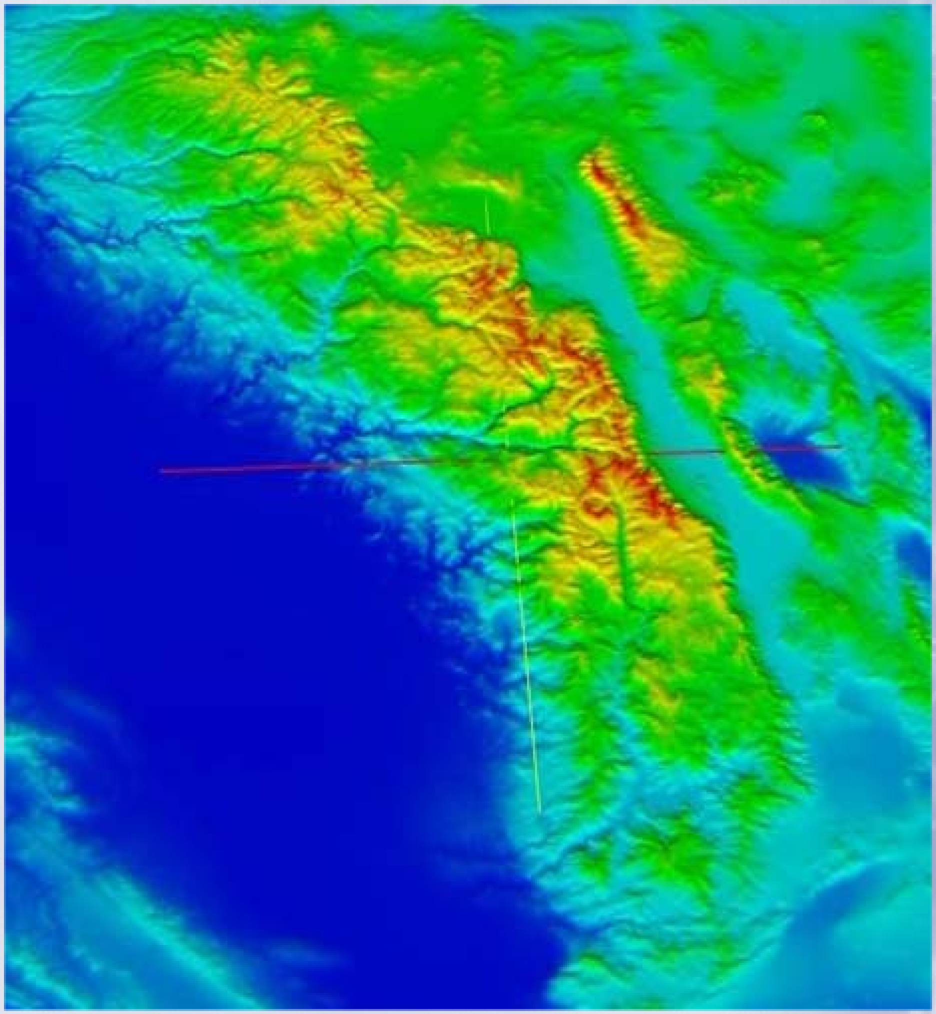
Outline

- Requirements for simulation of turbulence in complex geometries.
- Accuracy vs algorithmic complexity.
- Understanding numerical error – dissipative and dispersive components.
- 2nd order kinetic energy conserving schemes.
- Computational examples.
- Conclusions.

Numerical Requirements

- General boundary conditions.
- Curvilinear coordinate system.
- Arbitrary mesh spacing - structured or unstructured.
- Accuracy.
- Computational efficiency.



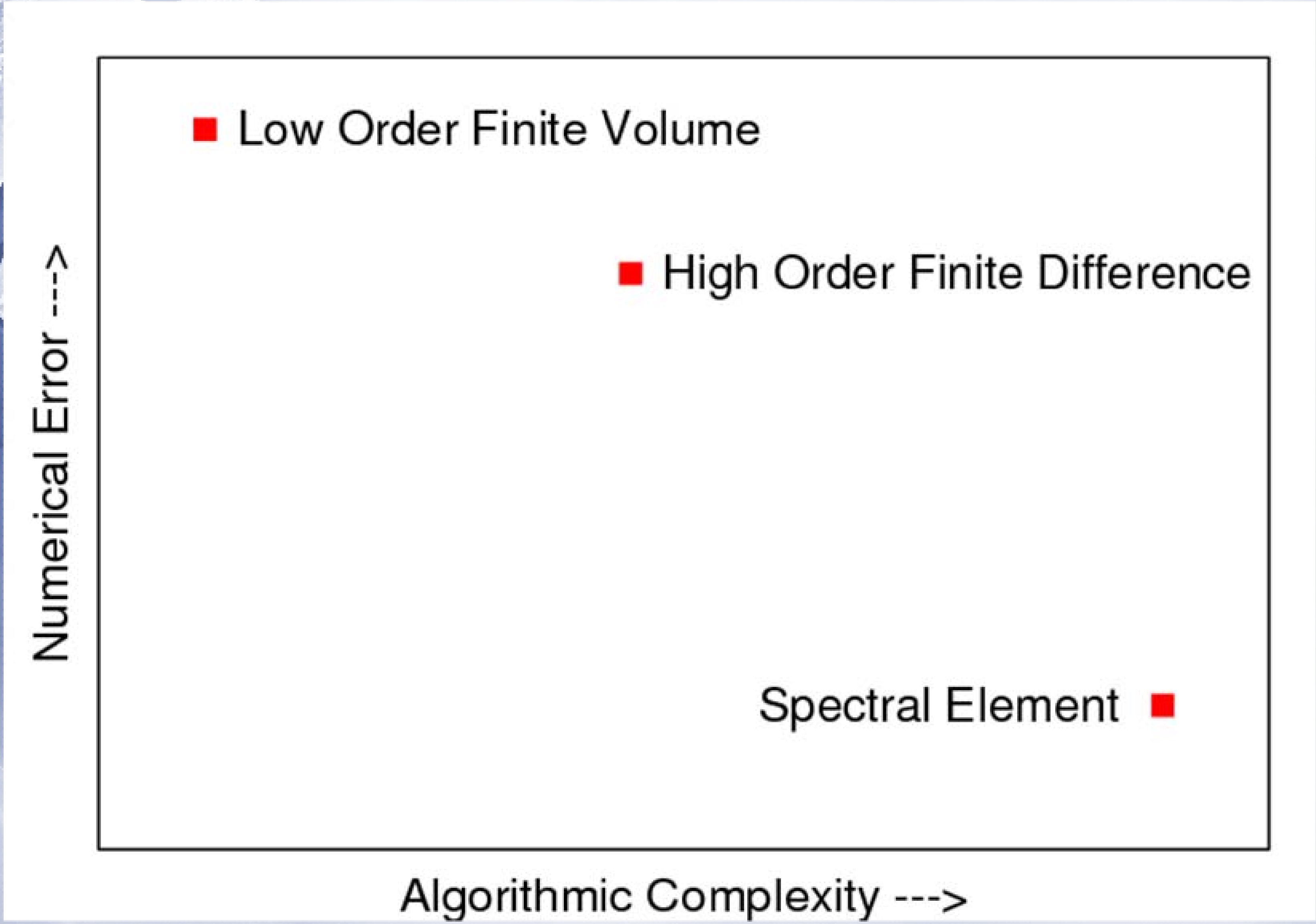
Candidate Algorithms

- ~~Spectral~~
- Spectral Element
- Finite Element
- Finite Volume
- Finite Difference

Issues to Consider

- Accuracy
  - Numerical dissipation
  - Numerical dispersion
- Algorithmic Complexity
  - Effort in coding, debugging, modification
  - Parallel efficiency
  - Numerical cost per grid point per time step

Error vs Complexity



Numerical Error

Consider the 1-d hyperbolic model problem in a periodic domain

$$\frac{\partial u}{\partial t} = c\frac{\partial u}{\partial x}$$

Upon Fourier transform

$$\frac{\partial \hat{u}}{\partial t} = ikc\hat{u}$$

The solution is

$$\hat{u}(k,t) = \hat{u}_0(k)\exp(ikct)$$

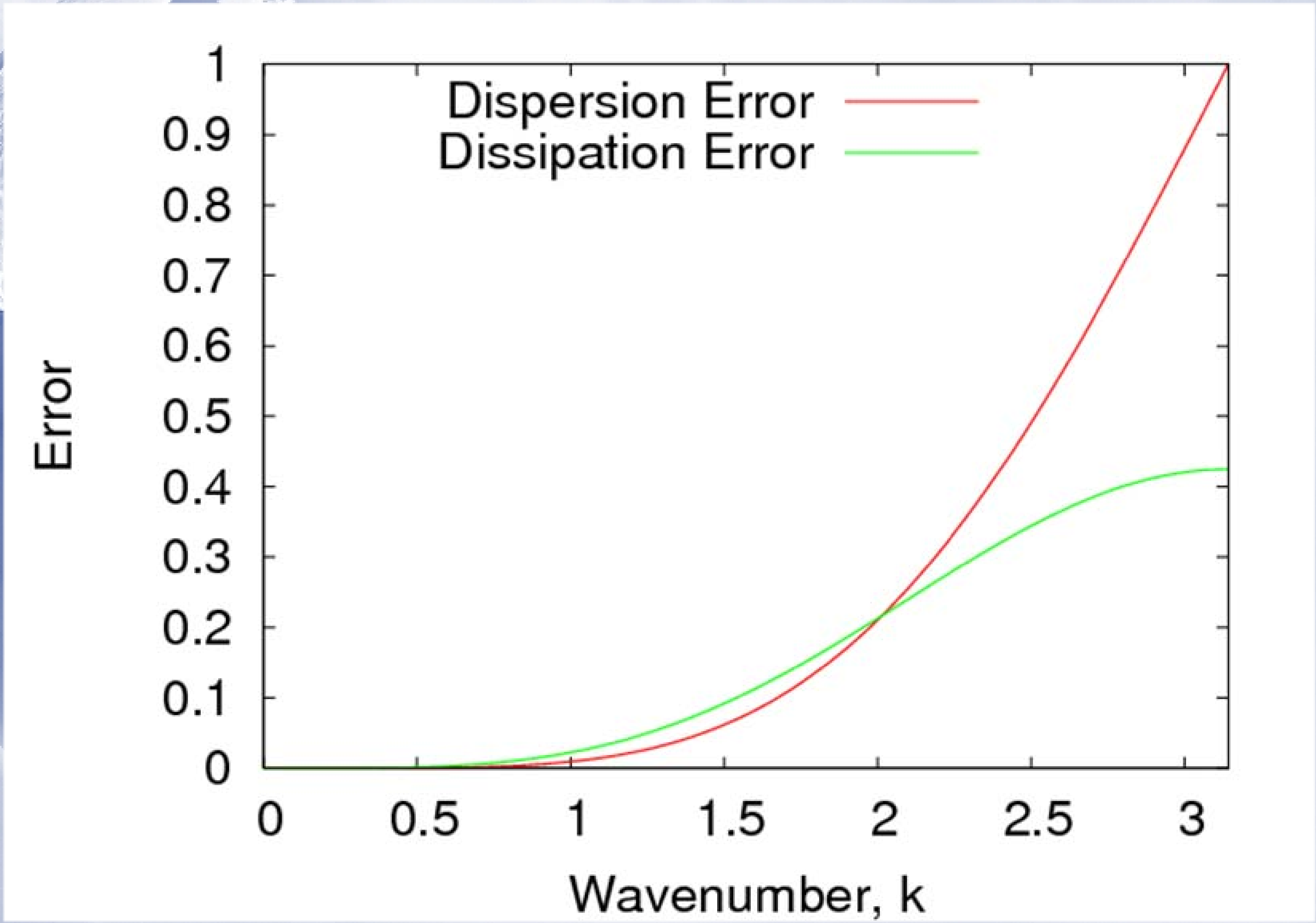
When discrete spatial operators are used, the Fourier space equation becomes

$$\frac{\partial \hat{u}}{\partial t} = ic\tilde{k}\hat{u}$$

where $\tilde{k}(k) = \tilde{k}_r(k) + i\tilde{k}_i(k)$ is the *modified wavenumber*. The solution to the discrete problem is

$$\hat{\tilde{u}}(k,t) = \underbrace{\exp(-\tilde{k}_i ct)}_{\text{dissipation}}\ \underbrace{\exp[i(\tilde{k}_r - k)ct]}_{\text{dispersion}}\ \underbrace{\hat{u}_0(k)\exp(ikct)}_{\hat{u}}$$

Error Components - 3rd Order Upwind



Centered Schemes

- Symmetric schemes have no dissipation error.
- These schemes are usually unstable for high Reynolds number flows.
- The problem is that they do not conserve kinetic energy even though mass, momentum, and total energy are conserved.
- Numerical dissipation (upwinding) is often used to mask the kinetic energy conservation problem. Dissipation is bad for turbulence!

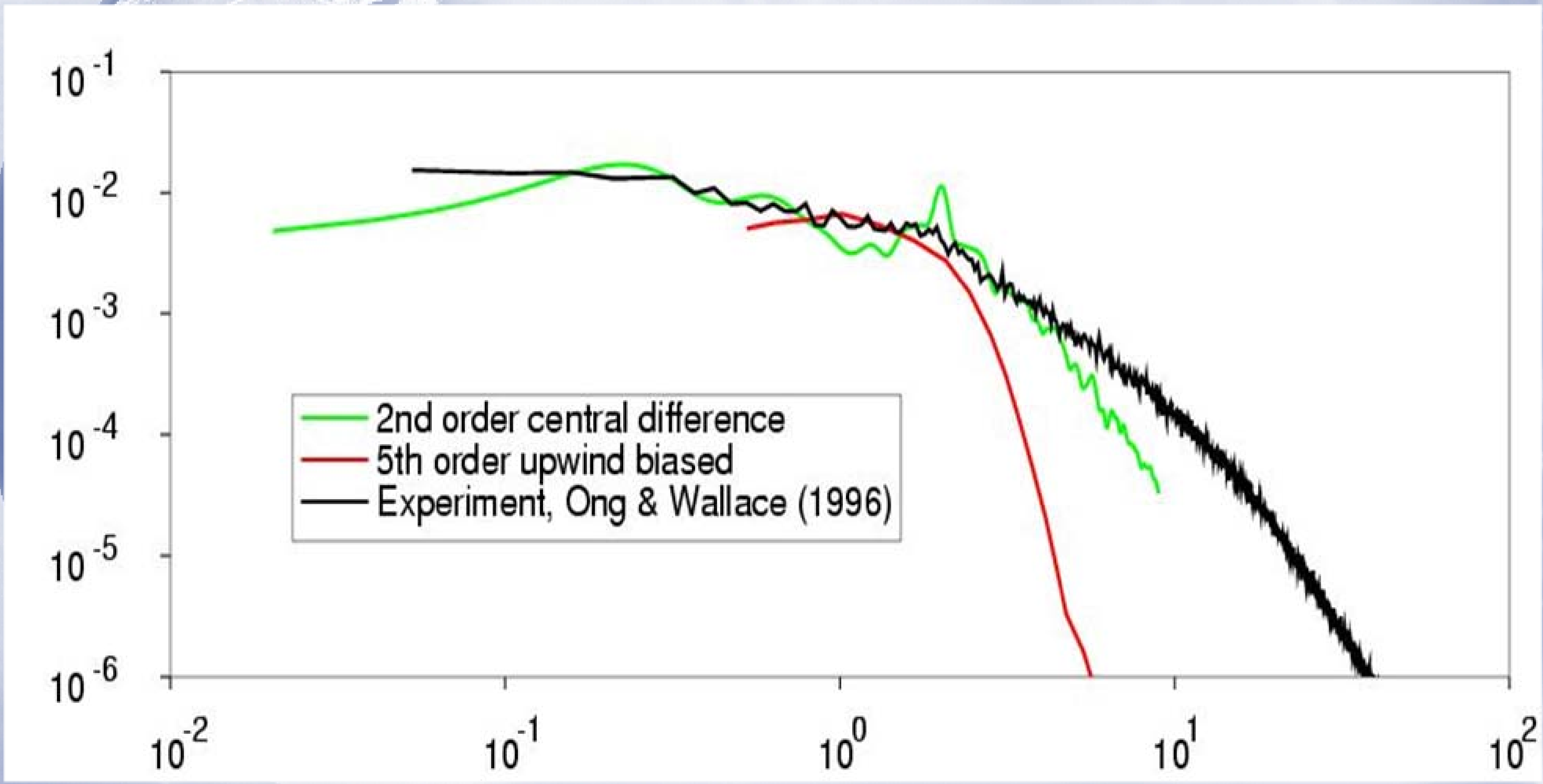
Kinetic Energy Conserving Schemes

- Through the correct use of averaging operators, symmetric differencing schemes can be made to conserve kinetic energy.
- These schemes are stable at arbitrary Reynolds number and have no numerical dissipation.
- 2nd order variants are easy to derive and code.
- Extension to higher orders is difficult and may impossible for certain boundary conditions.

Alternatives for Discrete Methods

1. Use an upwind scheme. Although the work increases, the order can be increased arbitrarily.
2. Use a 2nd order kinetic energy conserving scheme. What about dispersion error in this case?

Dissipation vs Dispersion - Turbulent Wake



Effects of Numerical Dissipation

- Numerical dissipation removes significant energy at small scales, overriding the turbulence cascade mechanism.
- There is overwhelming evidence to suggest that dissipative schemes are very poorly suited for turbulence simulation.
- This is especially true for Large Eddy Simulation (LES) where there is supposed to be significant energy at the grid scale.

Effects of Numerical Dispersion

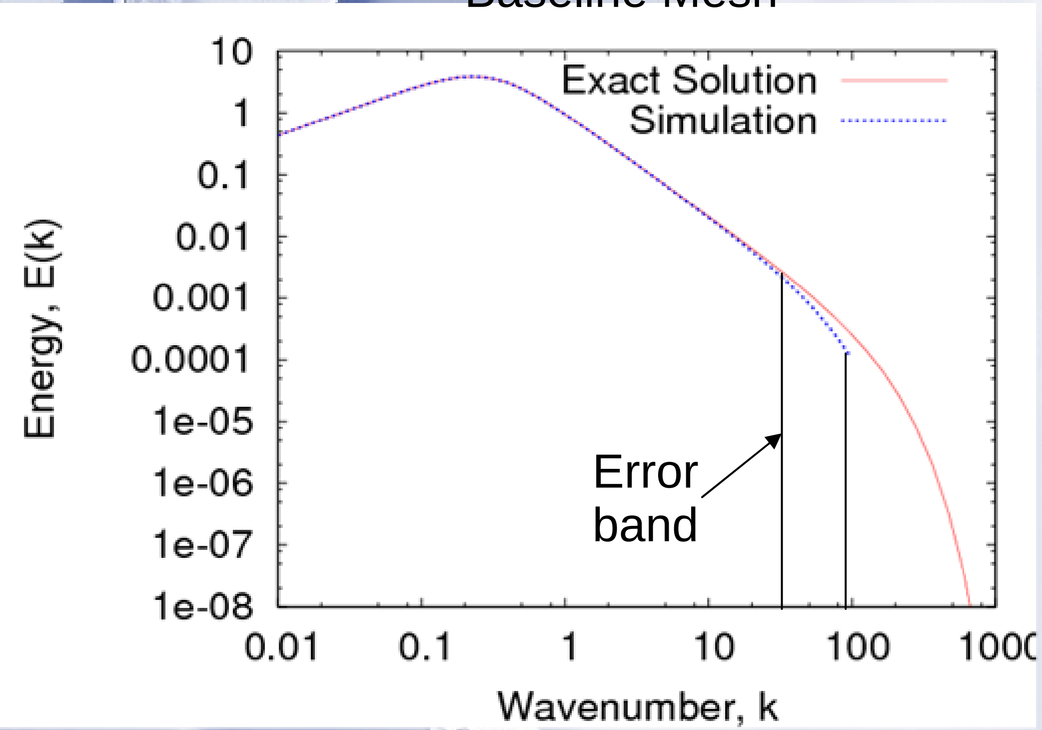
- The effects of dispersion error are much more subtle.
- Dispersion tends to “scramble” small scale structures which indirectly interferes with the turbulent cascade mechanism.
- There is considerable evidence to suggest that turbulence is surprisingly forgiving of this type of error.

Minimizing Dispersion Error

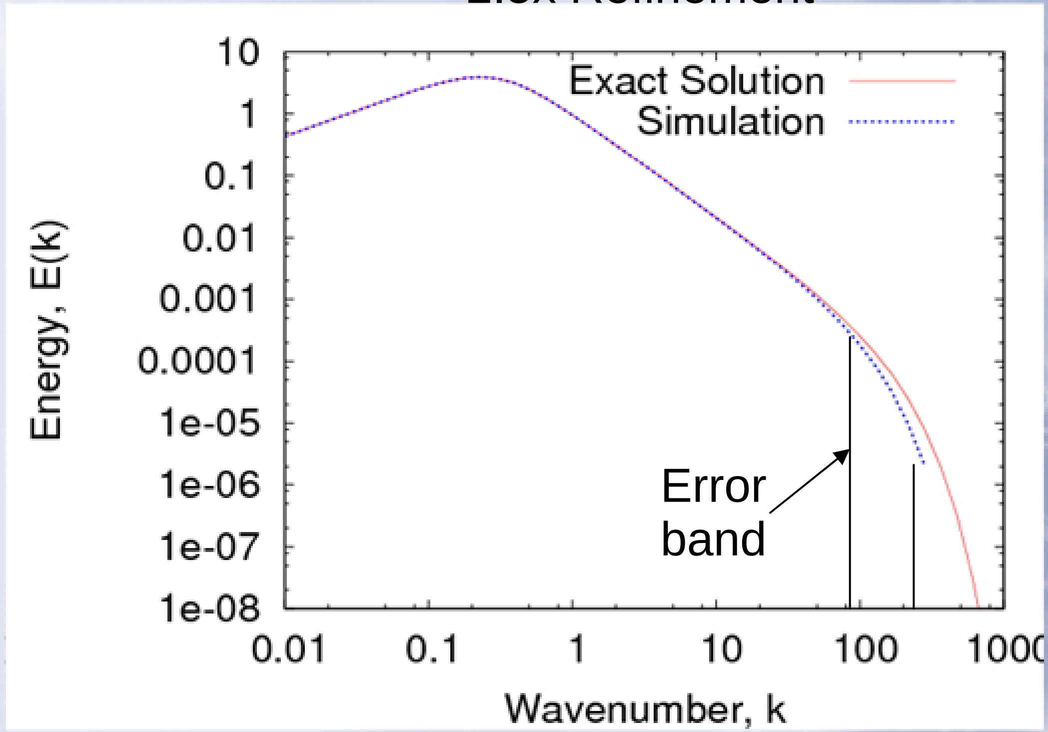
- We can minimize the effects of dispersion error by simply refining the mesh.
- Petascale computing combined with the numerically efficient 2nd order algorithm allows us to compute with 10^{11}-10^{13} mesh points.
- Although error is still present, it is pushed to a less energetic portion of the solution.
- These error-contaminated very small scales are still effective at transferring and dissipating energy.

Mesh Refinement Shifts Error to Smaller Scales

Baseline Mesh



2.5x Refinement

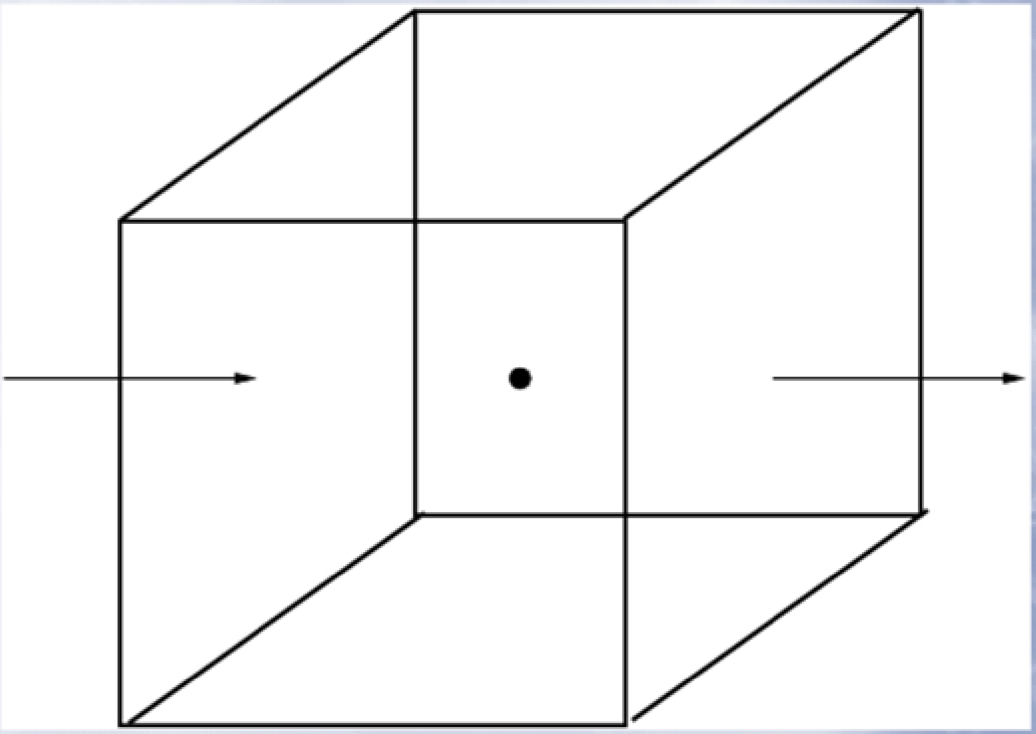


Experience with 2nd Order Schemes

- For DNS mesh refinement by a factor of 2 yields results that compare well with spectal methods (Choi and Moin 1990).
- For LES, factors of 2-3 are required (Lund 1995).

2nd Order Finite Volume Method

- Interpolate velocity from centers to face.
- Project velocity onto the face normal to compute fluxes.
- Balance fluxes to get time rates of change.



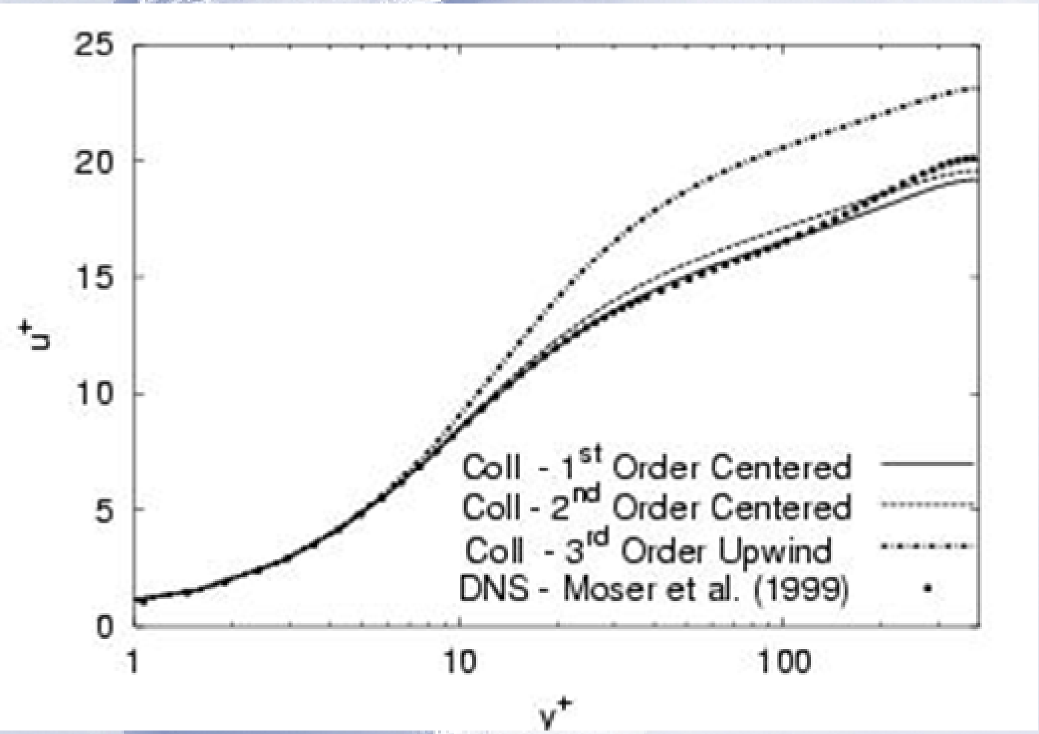
Advantages of 2nd order F.V.

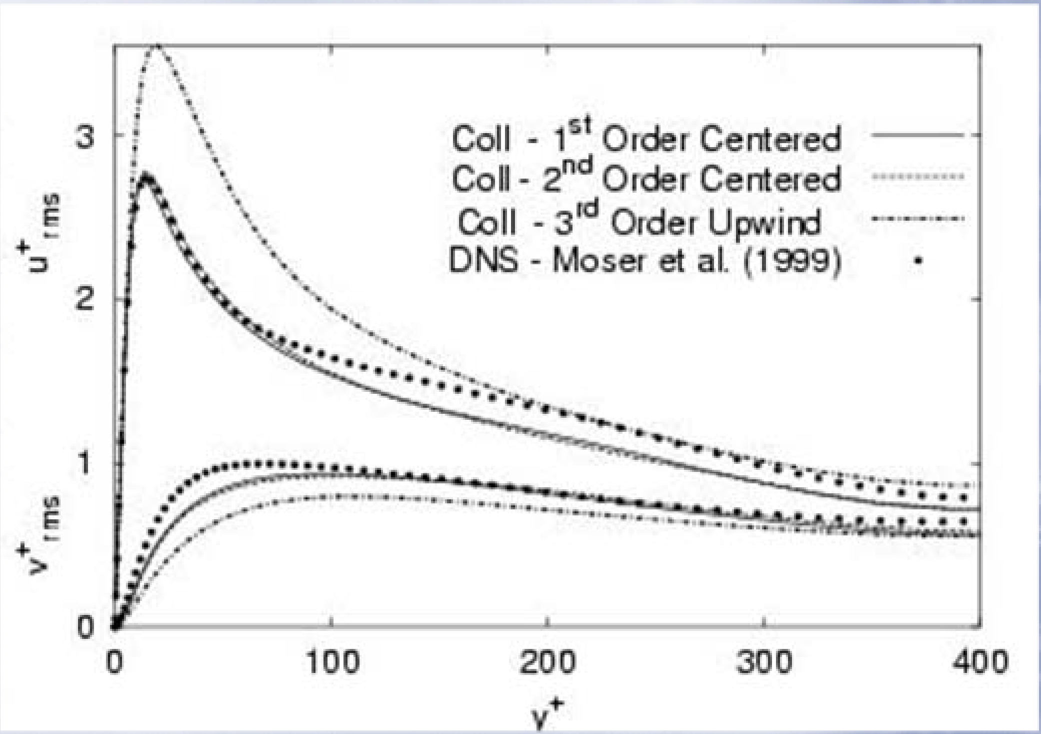
- Fully conservative (mass, momentum, kinetic energy).
- No coordinate transformation required - Cartesian velocity components are the solution variables.
- Very easy to understand, code, and modify.
- Very easy to achieve high parallel efficiency.
- Can be extended to irregular, unstructured meshes.

Sample Simulations

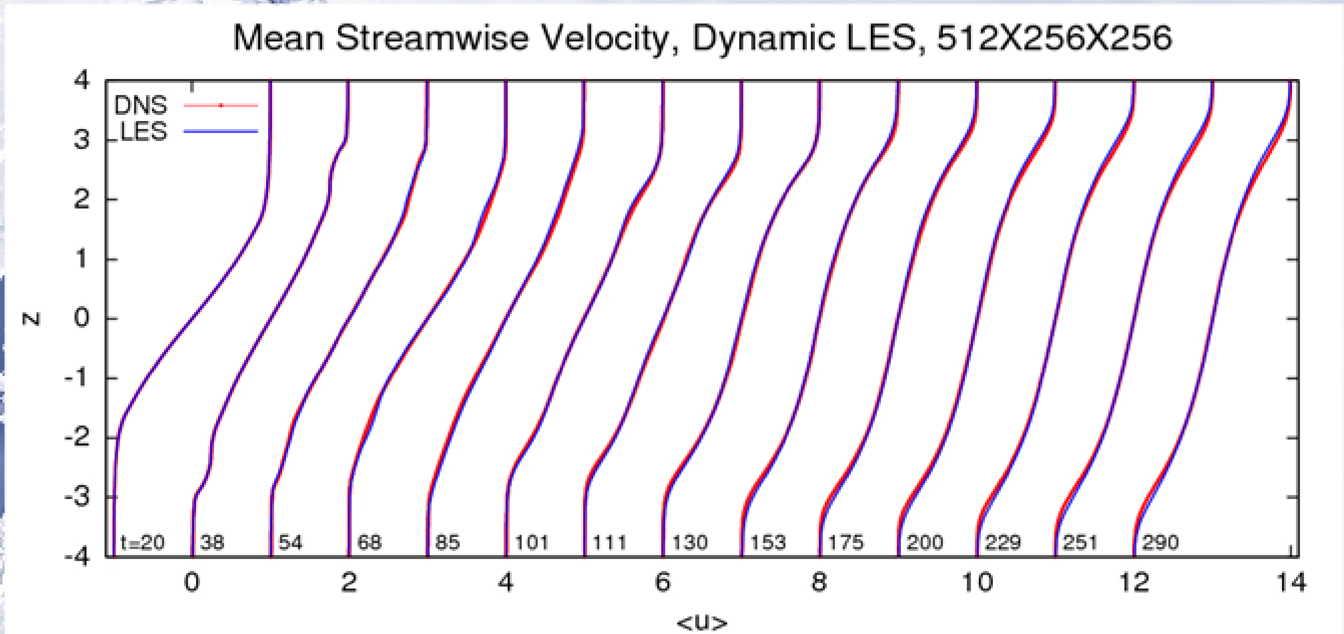
- Turbulent channel flow.
- Kelvin-Helmholtz instability.
- Asymmetric diffuser.
- Circular cylinder wake.
- Jet engine compressor.

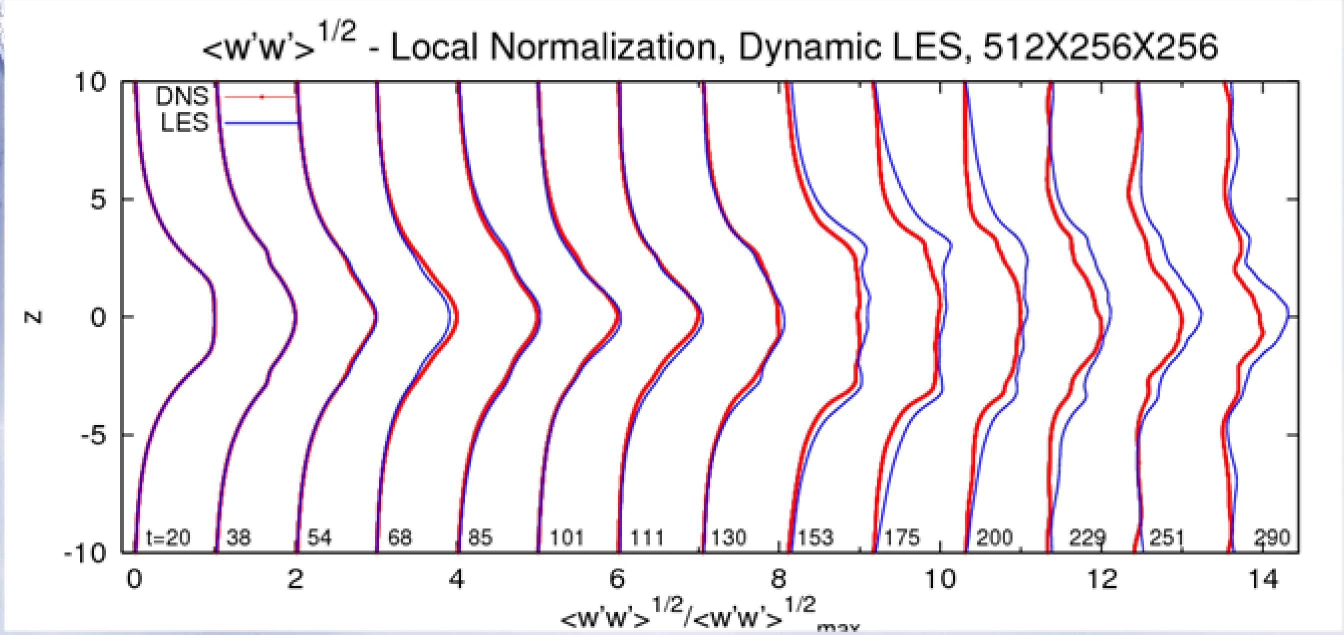
Turbulent Channel Flow R_t=390





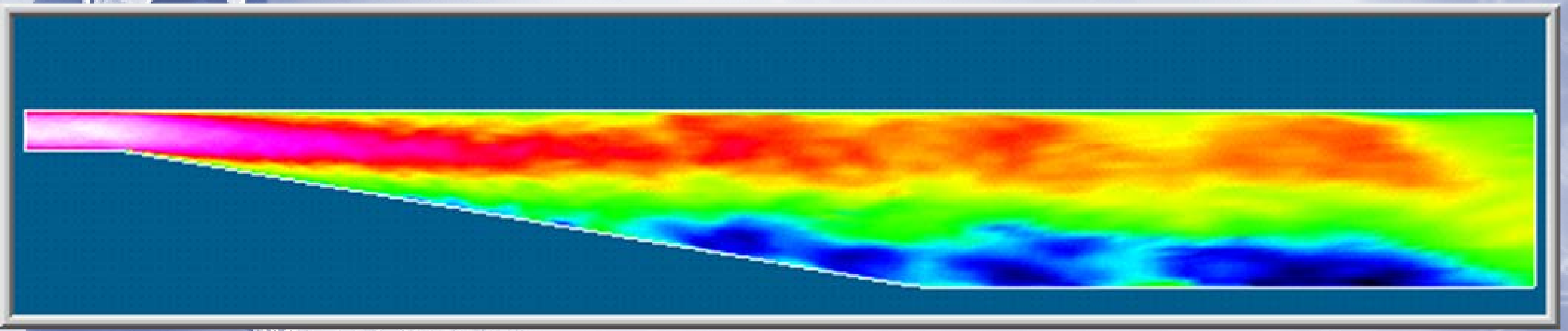
Kelvin-Helmholtz Instability Re=2500





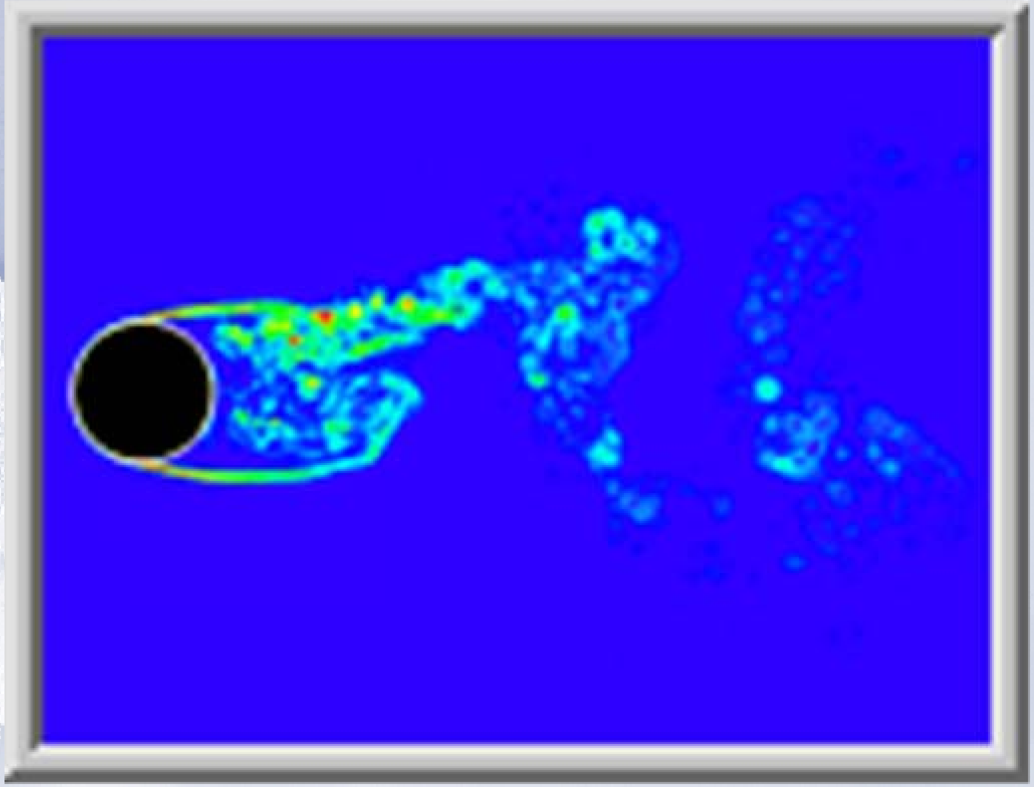
Asymmetric Diffuser

Kaltenbach et al. 1999



Cylinder Wake - Re=3900

Krevchenko et al. 1998



Jet Engine Compressor

Schluter et al. 2002

QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.

Conclusions

- 2nd order kinetic energy conserving schemes are surprisingly well-suited for turbulence simulation.
- The algorithms are easy to understand, program, and modify.
- 2-3 times increase in grid resolution give solutions that compare well with spectral methods.
- These algorithms make increasing sense as computers become larger and faster.