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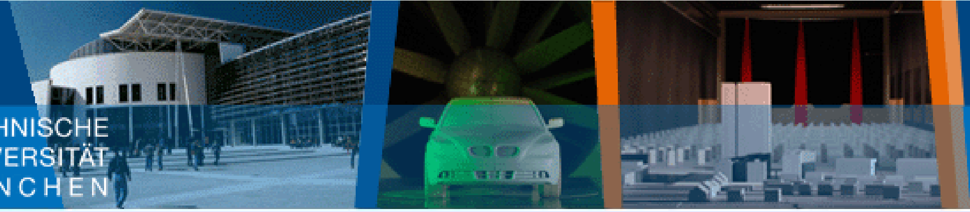

Lehrstuhl für Aerodynamik und Strömungsmechanik

Stochastic subgrid-scale estimation and scale-separating schemes for Large-Eddy Simulation

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Chapters:

1. **LES modeling based on subgrid-scale estimation**

2. **Implicit SGS modeling by scale separation**

3. **Stochastic subgrid-scale estimation**

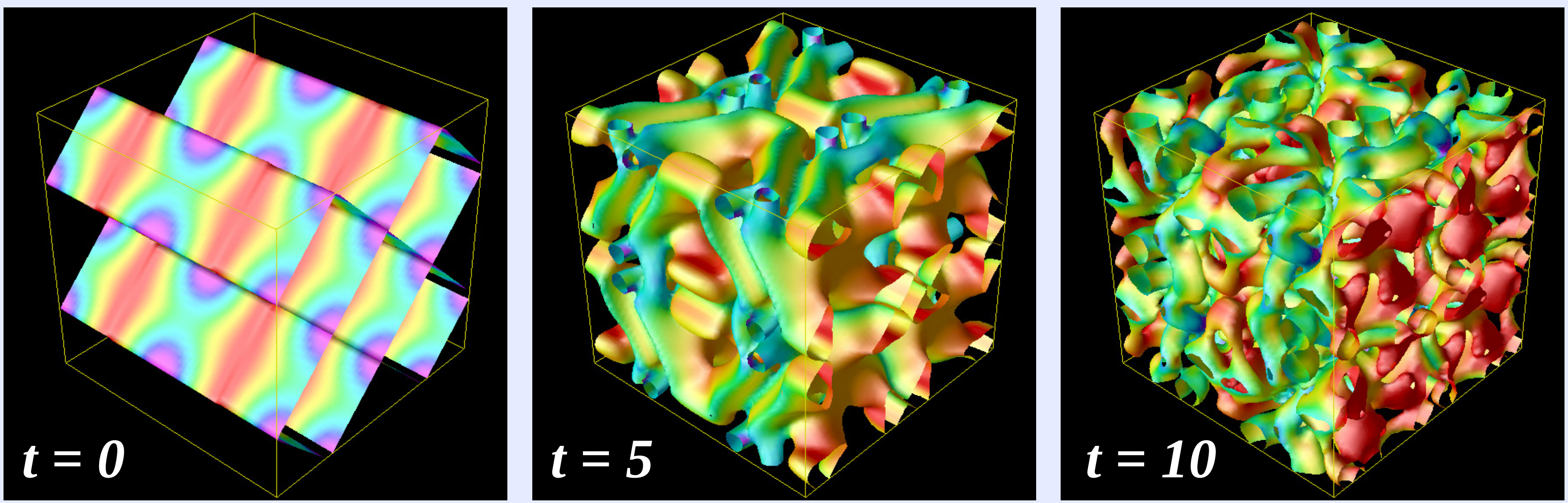
1. LES modeling based on subgrid-scale estimation

Numerical motivation of Large-Eddy Simulation:

Representation of flow evolution with reduced spatial dimensionality and bound on kinetic energy

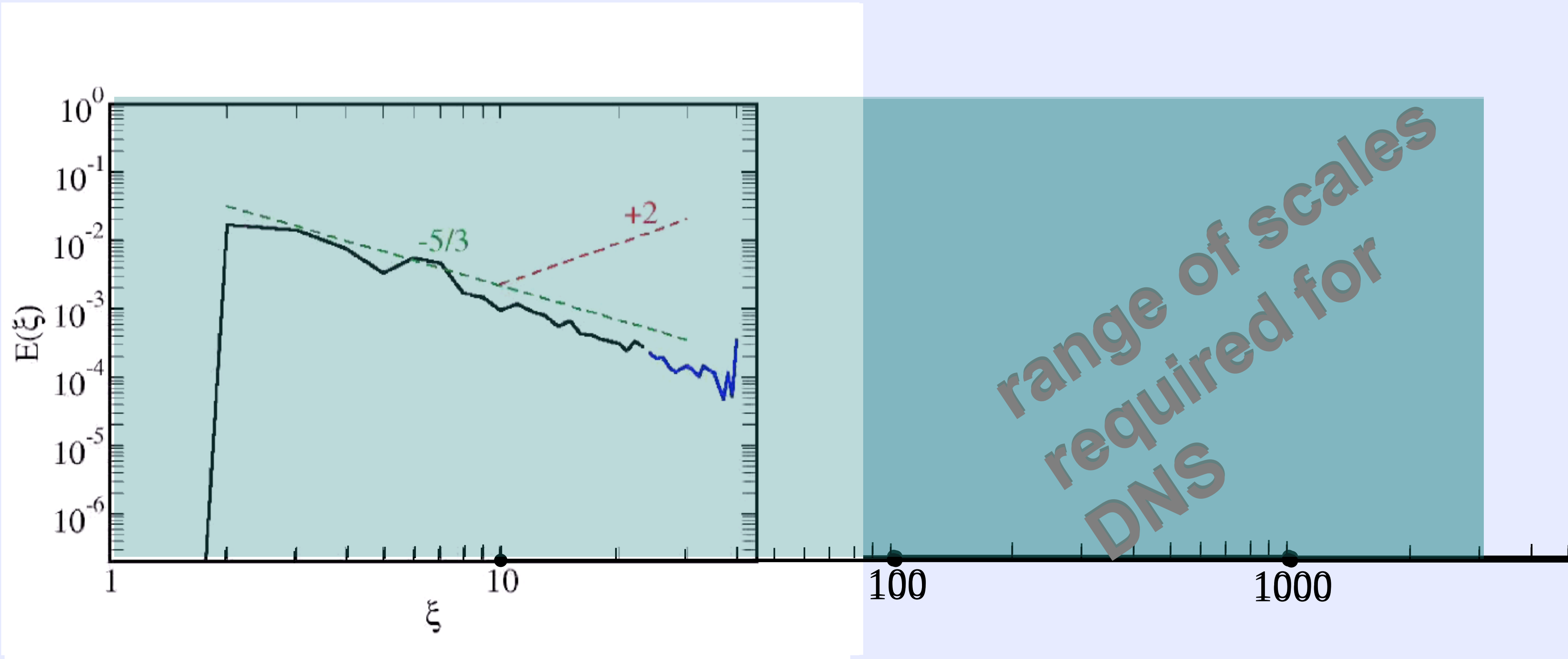
Consider as example the **3D Taylor-Green vortex**

- LES of 8 vortices in a triply periodic box with 64^3 cells
- visualization of time evolution at Re=400 (second-invariant criterion)

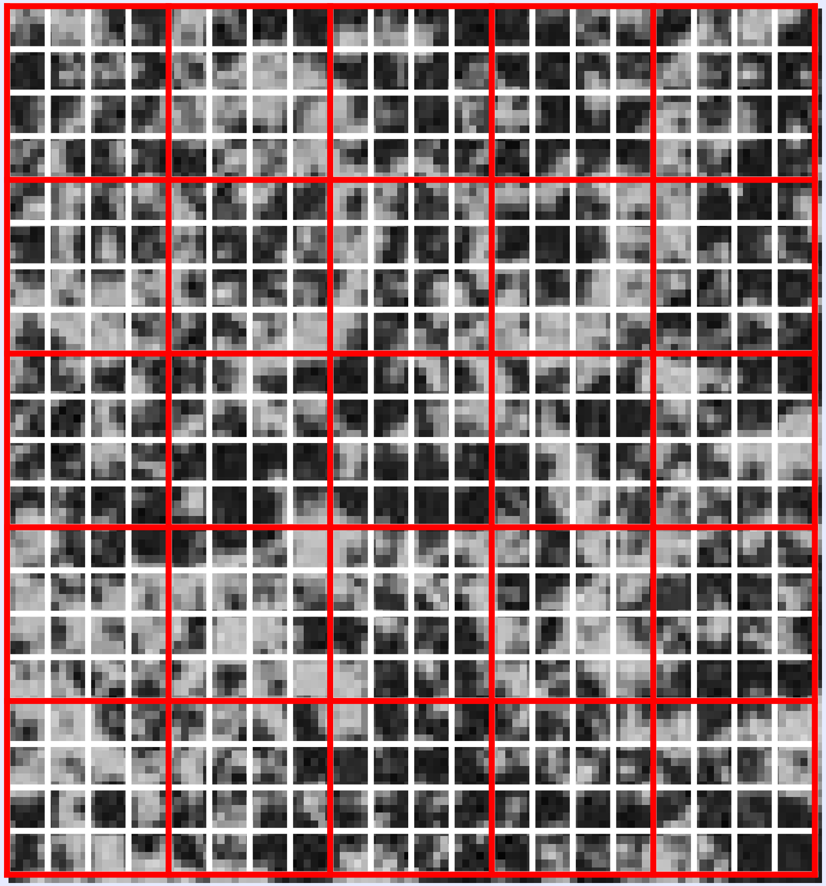


1. LES modeling based on subgrid-scale estimation

- evolution of scales – transition to isotropic turbulence for Re=3000
- subgrid-scale model with proper SGS energy transfer



1. LES modeling based on subgrid-scale estimation



Consider a generic conservation law governing the turbulent-flow evolution:

$$\frac{\partial}{\partial t} u + \frac{\partial}{\partial x} F(u) = 0$$

Assume that an "exakt" solution (DNS) u is obtained on the white grid.

The objective of LES is to compute an accurate solution on the coarser grid (red), the filtered solution:

$$u_N = G_N * u$$

1. LES modeling based on subgrid-scale estimation

Evolution equation for the filtered solution:

$$G_N * \left(\frac{\partial}{\partial t} u + \frac{\partial}{\partial x} F(u) \right) = \frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} F_N(u) = 0$$

$$\Rightarrow \frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} F_N(u_N) = \mathcal{G}_{SGS}$$

The SGS resdiual is not closed (involves unavailable information), requires modeling:

$$\mathcal{G}_{SGS} = \frac{\partial}{\partial x} F_N(u_N) - \frac{\partial}{\partial x} F_N(u)$$

Let now $u_N = G_N * u$ be the cell averaged solution of the Finite-Volume-semi-discretized conservation law:

$$\frac{\partial}{\partial t} u_N + \frac{\delta}{\delta x} \tilde{F}_N(\tilde{u}_N) = 0 \quad \text{where} \quad \tilde{u}_N \approx u$$

The Modified Differential Equation for u_N is then

$$\frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} F_N(u_N) = \mathcal{G}_{num}$$

where

$$\mathcal{G}_{num} = \frac{\partial}{\partial x} F_N(u_N) - \frac{\delta}{\delta x} \tilde{F}_N(\tilde{u}_N)$$

is the (spatial) truncation error.

1. LES modeling based on subgrid-scale estimation

Analogy between the **Finite-Volume discretization** of the conservation law and the **LES evolution equation** :

Filtered conservation law (LES)

$$\frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} F_N\left(u_N\right) = \mathcal{G}_{SGS}$$

filtered grid function — SGS residual

$$\mathcal{G}_{SGS} = \frac{\partial}{\partial x} F_N\left(u_N\right) - \frac{\partial}{\partial x} F_N\left(u\right)$$

Discretized conservation law (FV)

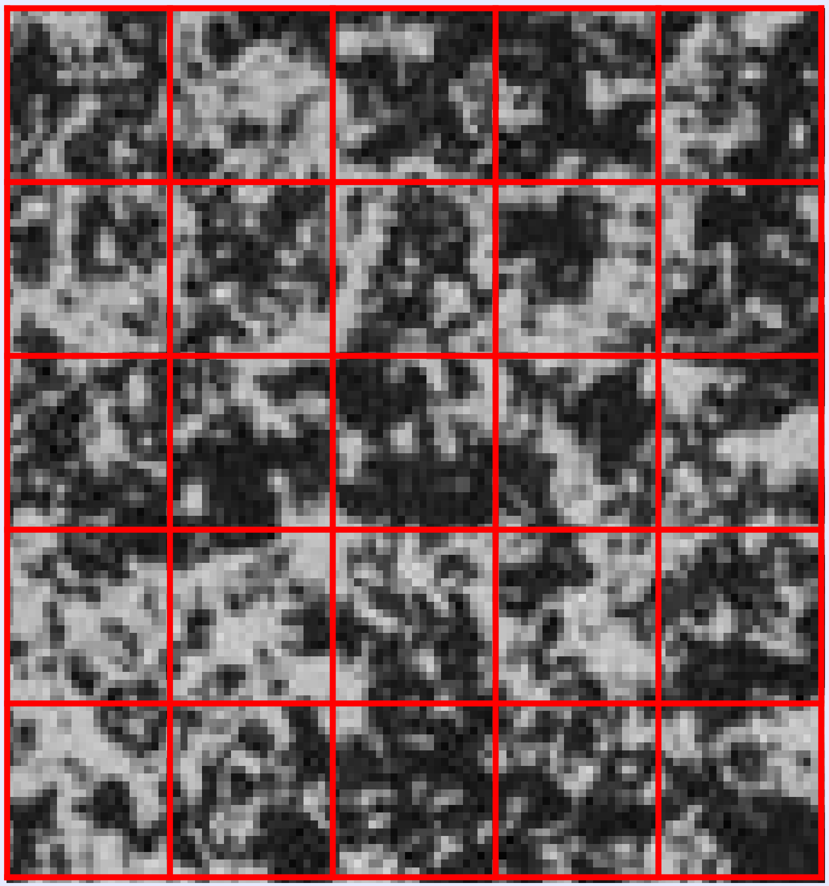
$$\frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} F_N\left(u_N\right) = \mathcal{G}_{num}$$

discrete solution — truncation error

$$\mathcal{G}_{num} = \frac{\partial}{\partial x} F_N\left(u_N\right) - \frac{\delta}{\delta x} \tilde{F}_N\left(\tilde{u}_N\right)$$

1. LES modeling based on subgrid-scale estimation

Interference of truncation error and SGS residual:



If we discretize the **LES equations** we have as modified equation:

$$\frac{\partial}{\partial t} u_N + \frac{\partial}{\partial x} F_N\left(u_N\right) = \mathcal{G}_{SGS} + \mathcal{G}_{num}$$

If we are interested in a discrete solution where the grid size is not much smaller than characteristic flow scales $\mathcal{G}_{num}$ is not small.

In LES **truncation error and SGS model interfere**.

1. LES modeling based on subgrid-scale estimation

Two fundamentally different paradigms to *numerical* LES:

1. **Implicit LES:**

Synopsis: Numerical discretization and SGS model are connected

Constraint: $\mathcal{G}_{num} \overset{physical\ \ consistency}{\approx} \mathcal{G}_{SGS}$ so that truncation error acts as physically consistent SGS model

In practice:

- Physical consistency often “overlooked”
- Incorporation of physical consistency requires nonlinear discretization scheme
- Numerically “robust“

1. LES modeling based on subgrid-scale estimation

2. **Explicit LES:**

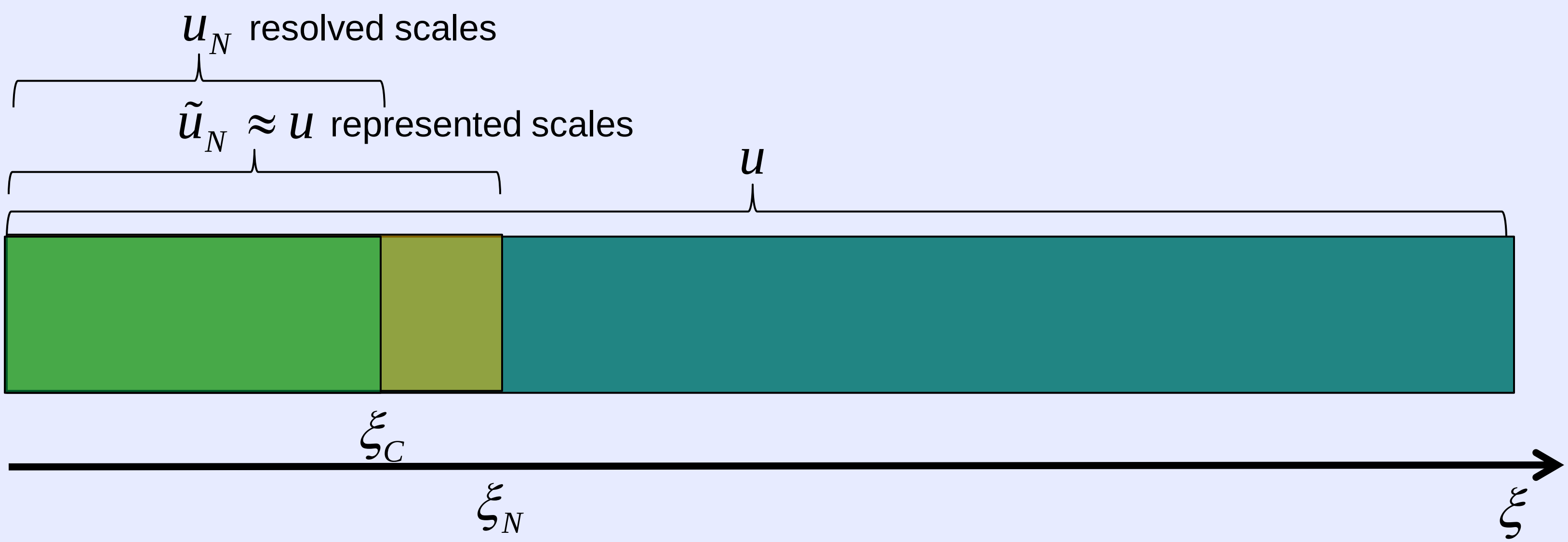
Synopsis: Numerical discretization and SGS model are independent

Constraint: $\left\| \mathcal{G}_{num} \right\| \ll \left\| \mathcal{G}_{SGS} \right\|$ so that the SGS has effect

In practice:

- Constraint rarely satisfied
- Explicit filter necessary for scale separation
- High-resolution discretization schemes necessary for small error throughout represented scales

1. LES modeling based on subgrid-scale estimation



Soft deconvolution: **approximate reconstruction** of non-resolved represented scales: $u_N \rightarrow \tilde{u}_N$

- recovers part of the SGS energy transfer
- improves prediction of anisotropy
- maintains tensorial structure of the exact SGS residual
- requires **additional regularization** for modeling the full SGS energy transfer

2. Implicit SGS modeling by scale separation

Approaches to Implicit LES can be classified (not comprehensive):

1. **Linear (i.e. CFL-number dependent) numerical dissipation:**
   - Multidirectional upwinding by Kawamura & Kuwahara 1984
2. **Limiter-based nonlinear dissipation:**
   - Flux-Corrected Transport by Boris & Grinstein 1992
   - Piecewise-Parabolic Method by Porter & Woodward 1998
3. **Nonlinear advection:**
   - MPDATA scheme by Margolin and Smolarkiewicz 1998
4. **Spectral regularization:**
   - Spectral Vanishing Viscosity by Tadmor 1990
5. **Nonlinear reconstruction:**
   - Approximate local deconvolution model by Hickel and Adams 2004,2006

2. Implicit SGS modeling by scale separation

How to impose criteria for physical consistency ?

- Direct manipulation of the truncation error, design of nonlinear scheme:
  - Adaptive local deconvolution model, WENO-type reconstruction (deconvolution), local Lax-Friedrichs-type numerical flux function for regularization, parameter adjusted for physical consistency
  - Not subject of today's presentation

  Several papers in *J. Comput. Phys. 2004, 2006, 2010, Phys. Fluids 2007, Int. J. Heat Fluid Flow 2010, several submitted*

- Indirect manipulation of the truncation error
  - A scheme that is physically consistent for turbulent subgrid-scales may be suboptimal for non-turbulent (genuine) subgrid scales

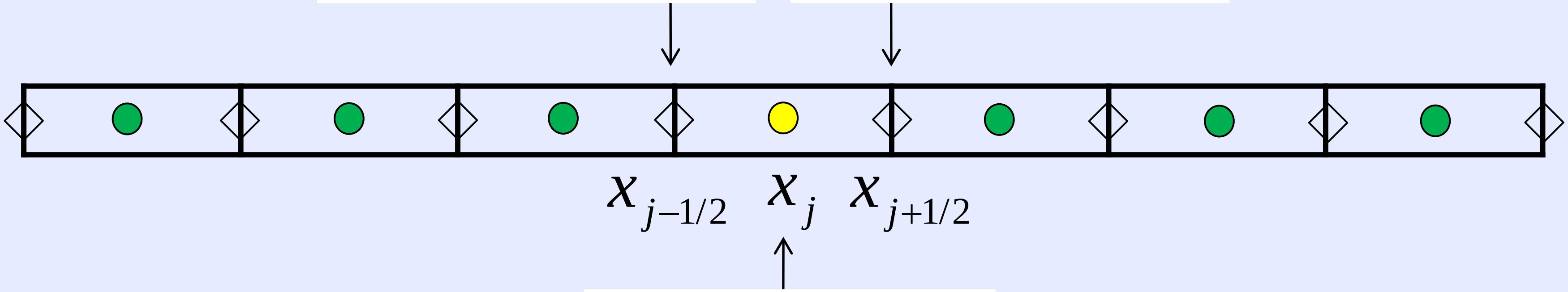
2. Implicit SGS modeling by scale separation

- Begin with good shock capturing scheme
- Consider 1D transport equation and Finite-Volume discretization

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} = 0$$

$$\frac{\partial u_j}{\partial t} + \frac{\tilde{F}_N\left(\tilde{u}_{j+1/2}\right) - \tilde{F}_N\left(\tilde{u}_{j-1/2}\right)}{h} = 0$$

$$\tilde{u}_{j-1/2} \approx u\left(x_{j-1/2}\right) \qquad \tilde{u}_{j+1/2} \approx u\left(x_{j+1/2}\right)$$

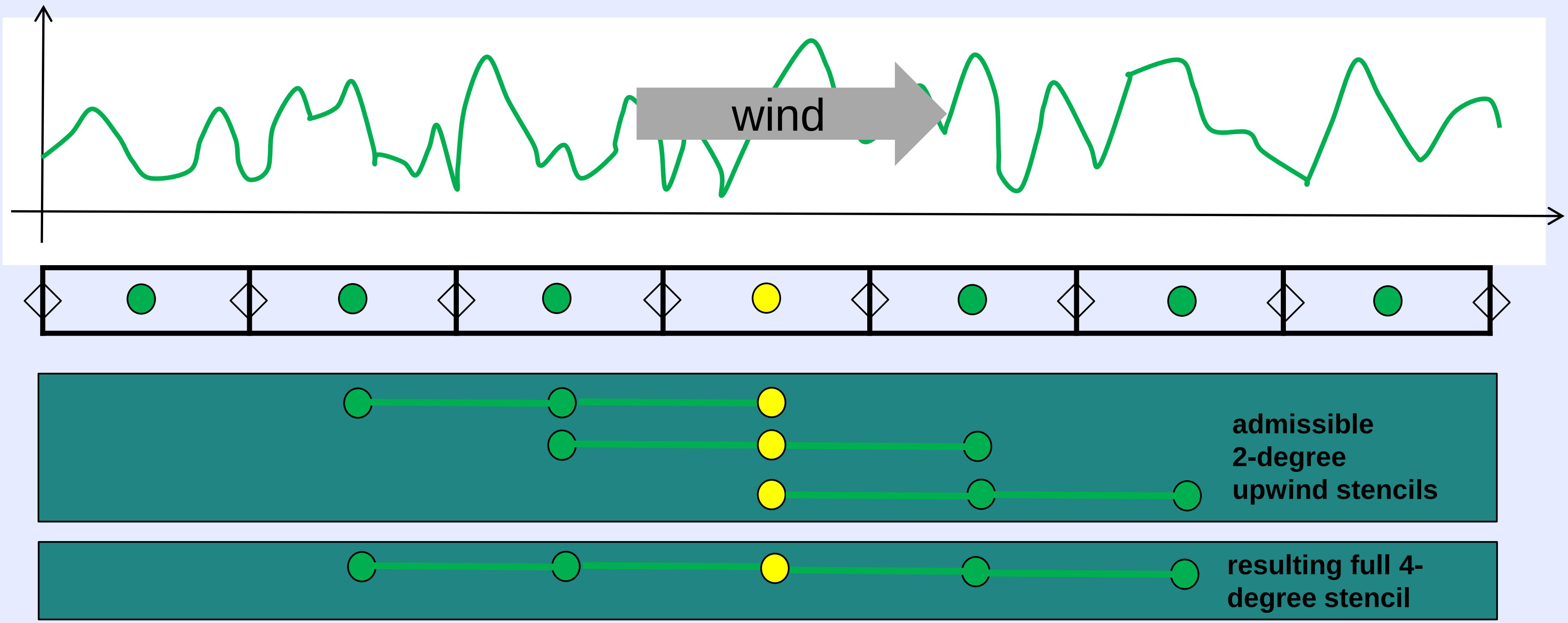


$$u_j \approx \left(G_N * u\right)\Big|_{x_j}$$

2. Implicit SGS modeling by scale separation

WENO reconstruction $\tilde{u}_{j+1/2} \approx \left(G_N^{-1} * u\right)\Big|_{x_j}$

- interpolation stencil is not unique and different stencils carry different smoothness and scale information



2. Implicit SGS modeling by scale separation

WENO5 reconstruction of the deconvolved filtered solution:

- Stencil contributions according to smoothess measures (the smoother the reconstruction polynomial on the stencil the larger the contribution)

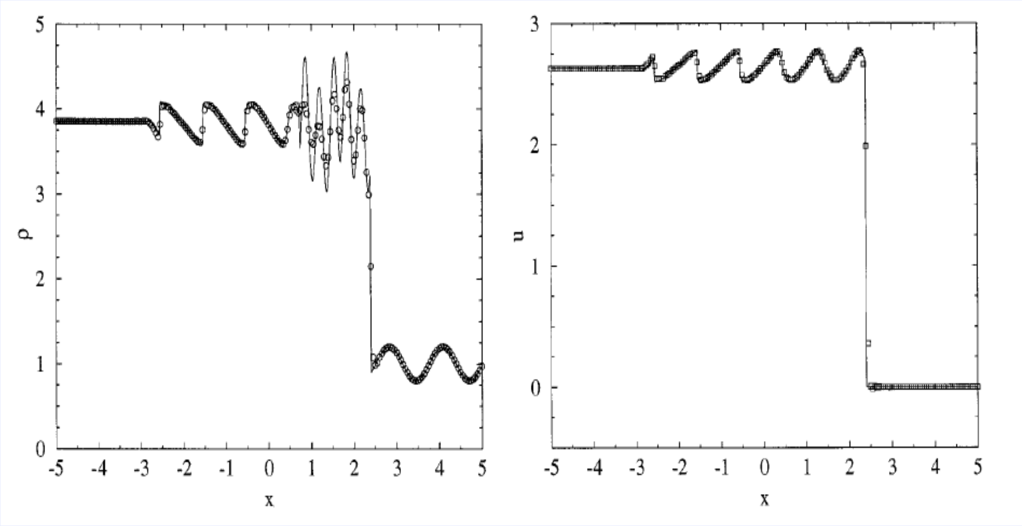
$$\omega_k = \frac{\alpha_k}{\sum_{k=0}^{2} \alpha_k}, \qquad \alpha_k = \frac{d_k}{(\beta_k + \epsilon)^q}.$$

$$\beta_k = \sum_{j=1}^{2} \Delta x^{2j-1} \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\frac{d^j}{dx^j} \hat{f}_k(x) \right)^2 dx,$$

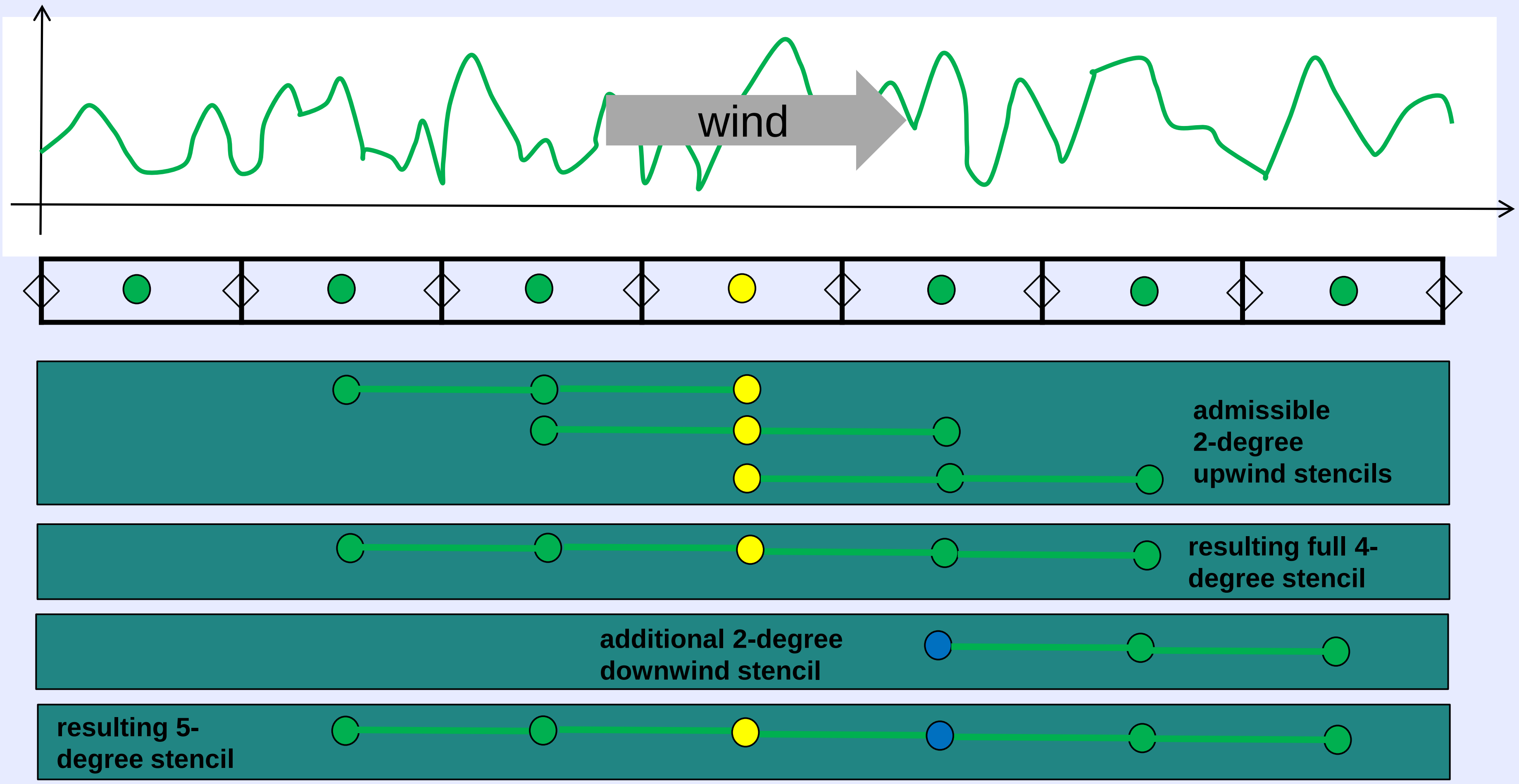
- Driven towards full-order (5-th order) upwind scheme when smoothness measure is uniform

- Rather dissipative anyway, “Shu-Osher problem”, here with Hybrid ENO5-compact-upwind scheme

  Adams & Shariff, JCP 1996



2. Implicit SGS modeling by scale separation



2. Implicit SGS modeling by scale separation

WENO-C6 reconstruction of the deconvolved filtered solution:

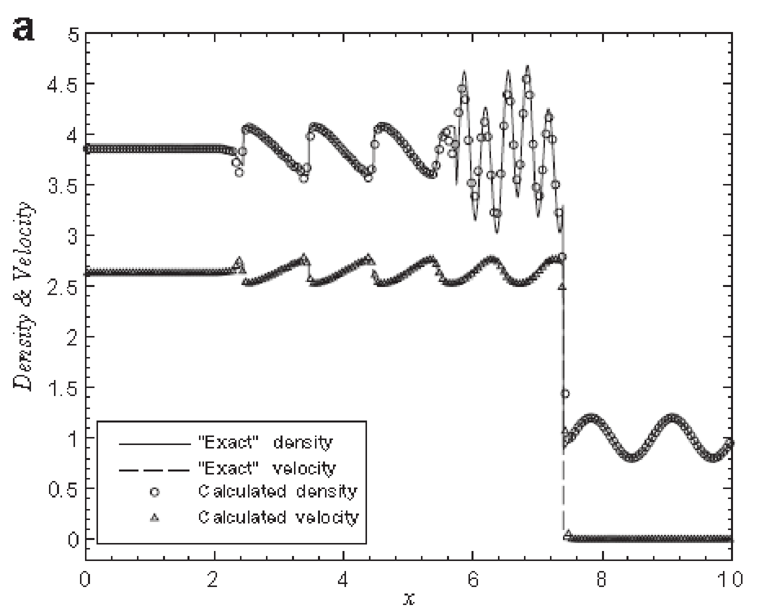
- Include downwind stencil to and drive towards full-order (6th-order) central scheme when smoothness measure is uniform

$$\omega_k = \frac{\alpha_k}{\sum_{k=0}^{3}\alpha_k}, \qquad \alpha_k = d_k\left(C + \frac{\tau_6}{\beta_k + \epsilon}\right),$$

- Preserve shock-capturing properties and reduce dissipation away from shock

Hu, Wang, Adams, JCP 2010

- Physically non-consistent for implicit SGS modeling, over-dissipative (inertial range not recovered up to the cutoff wavenumber)



2. Implicit SGS modeling by scale separation

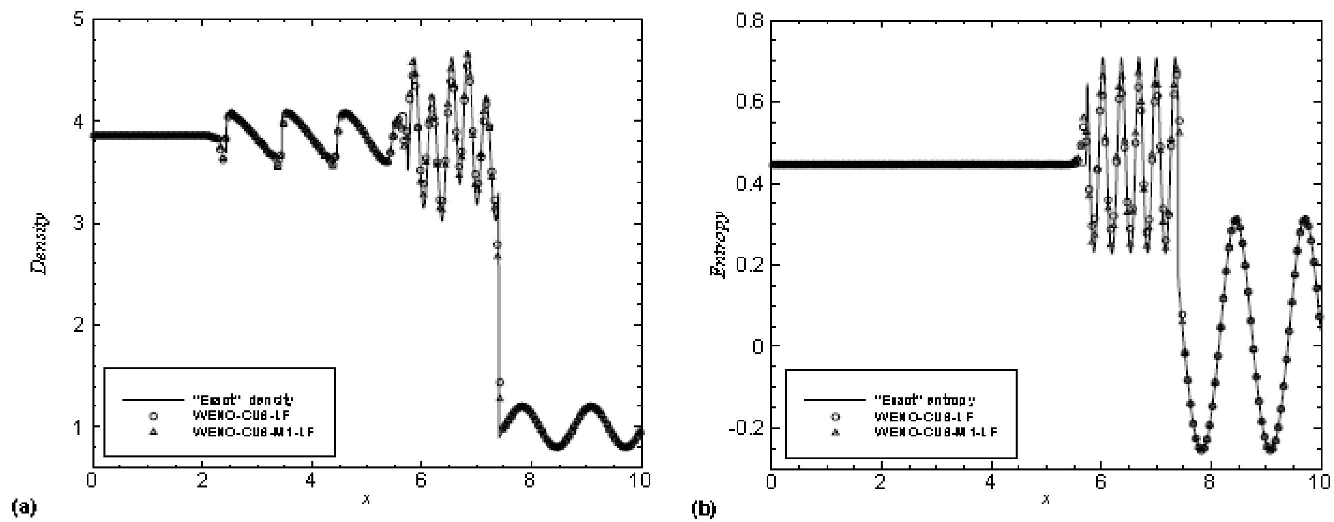
Scale separation WENO:

- Increase bias of central and upwind contributions (emphasize extrema)

  Hu, Adams, JCP 2011

$$\omega_r = \frac{\alpha_r}{\sum_{r=0}^{3} \alpha_r}, \quad \alpha_r = d_r \left(C_q + \frac{\tau^6}{\beta_r^3 + \epsilon \Delta x^2} \right)^q$$

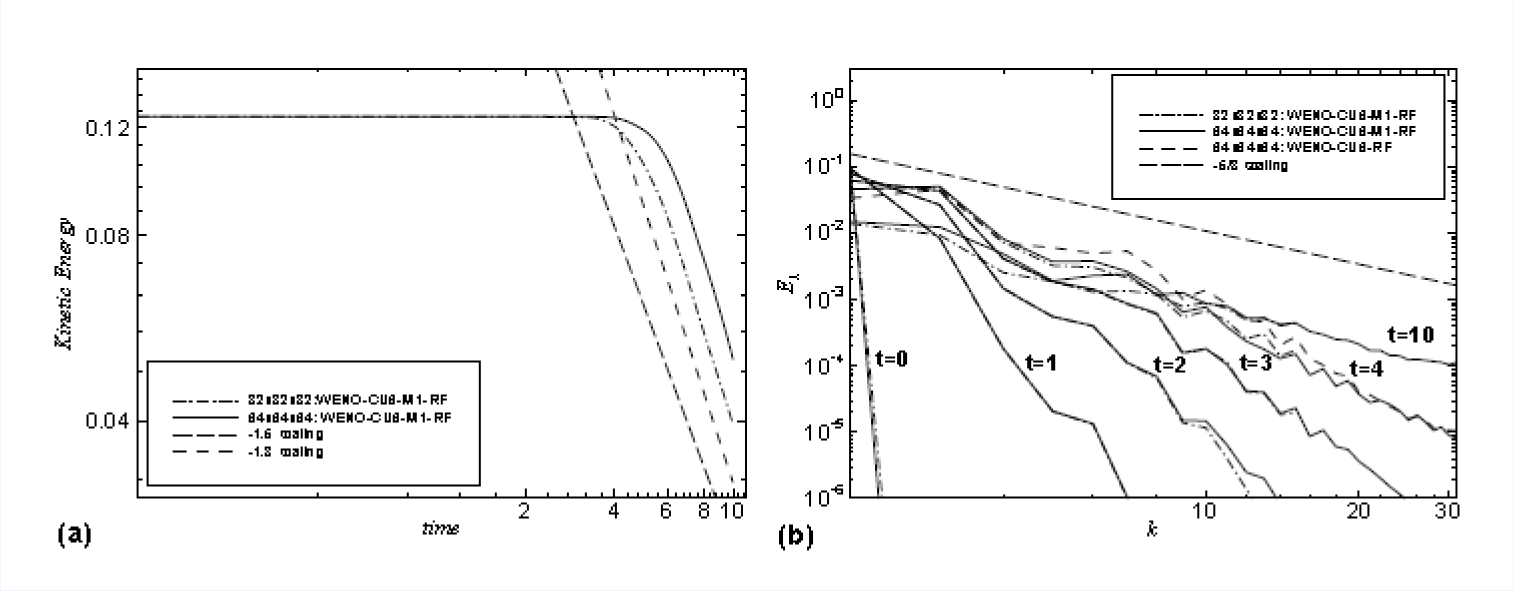
- Shock-capturing properties (essentially) preserved



2. Implicit SGS modeling by scale separation

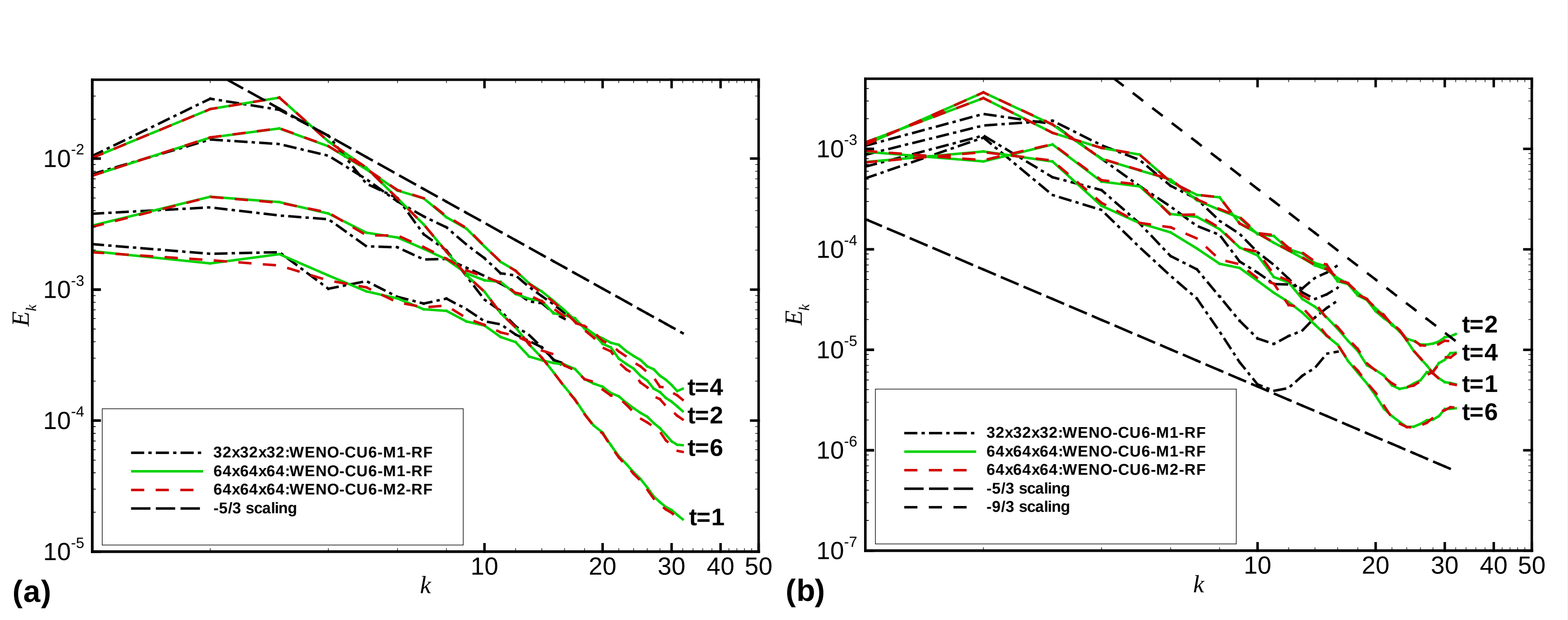
Scale separation WENO:

- Physically consistent prediction of low-Mach-number isotropic turbulence: Evolution of 3D-Taylor-Green vortex at infinite Reynolds number

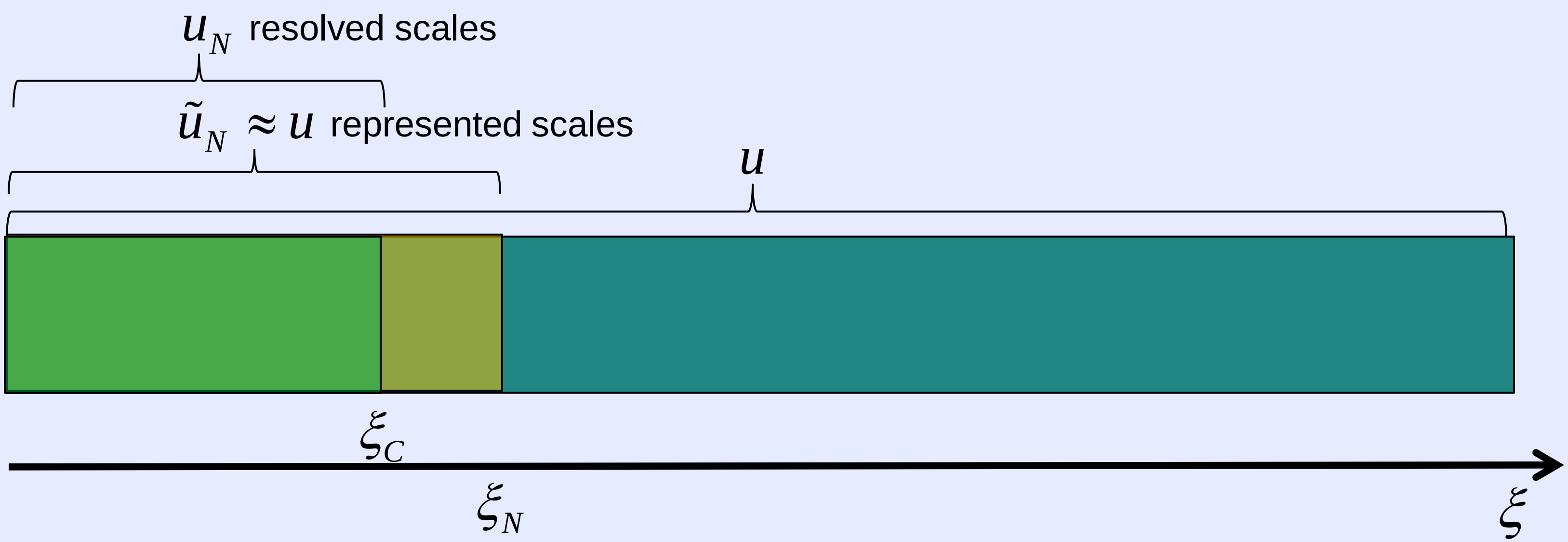


Scale separation WENO:

- Extension to compressible turbulence (pseudo-sound range)



3. Stochastic subgrid-scale estimation



Hard deconvolution: **direct reconstruction / estimation** of non-resolved represented scales: $u_N \rightarrow \tilde{u}_N$

- requires addditional model
- for computational efficiency only possible on limited scale range
- full SGS energy transfer needs to be modeled

3. Stochastic subgrid-scale estimation

Reconsider explicit LES by the approximate deconvolution model

Stolz, Adams, Phys. Fluids 1999

- Linear deconvolution / reconstruction operator
- Requires clear scale separation: resolved – non-resolved/represented – non-represented
- Requires small numerical truncation error on the range of represented scales

$$\frac{\partial}{\partial t}\bar{u}_N + \frac{\partial}{\partial x}F_N\left(\bar{u}_N\right) = \mathcal{G}_{SGS}$$

$$\mathcal{G}_{SGS} = \frac{\partial}{\partial x}F_N\left(\bar{u}_N\right) - \frac{\partial}{\partial x}\overline{F_N\left(\tilde{u}_N\right)}$$

- Reconstruction of an approximation of the filtered field by a (linear) regularized approximate inverse of the filter operator

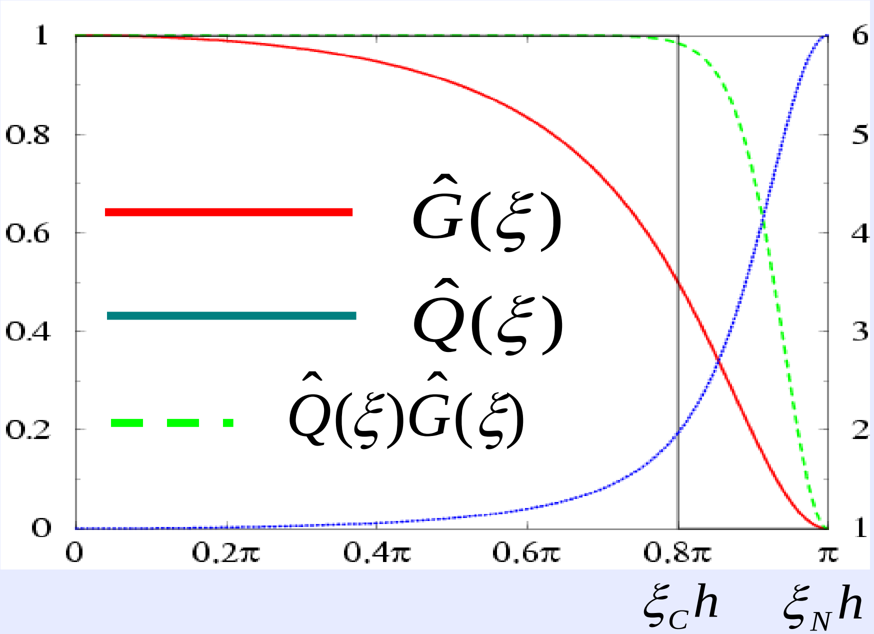
$$\tilde{u}_N = Q * \bar{u}_N$$

3. Stochastic subgrid-scale estimation

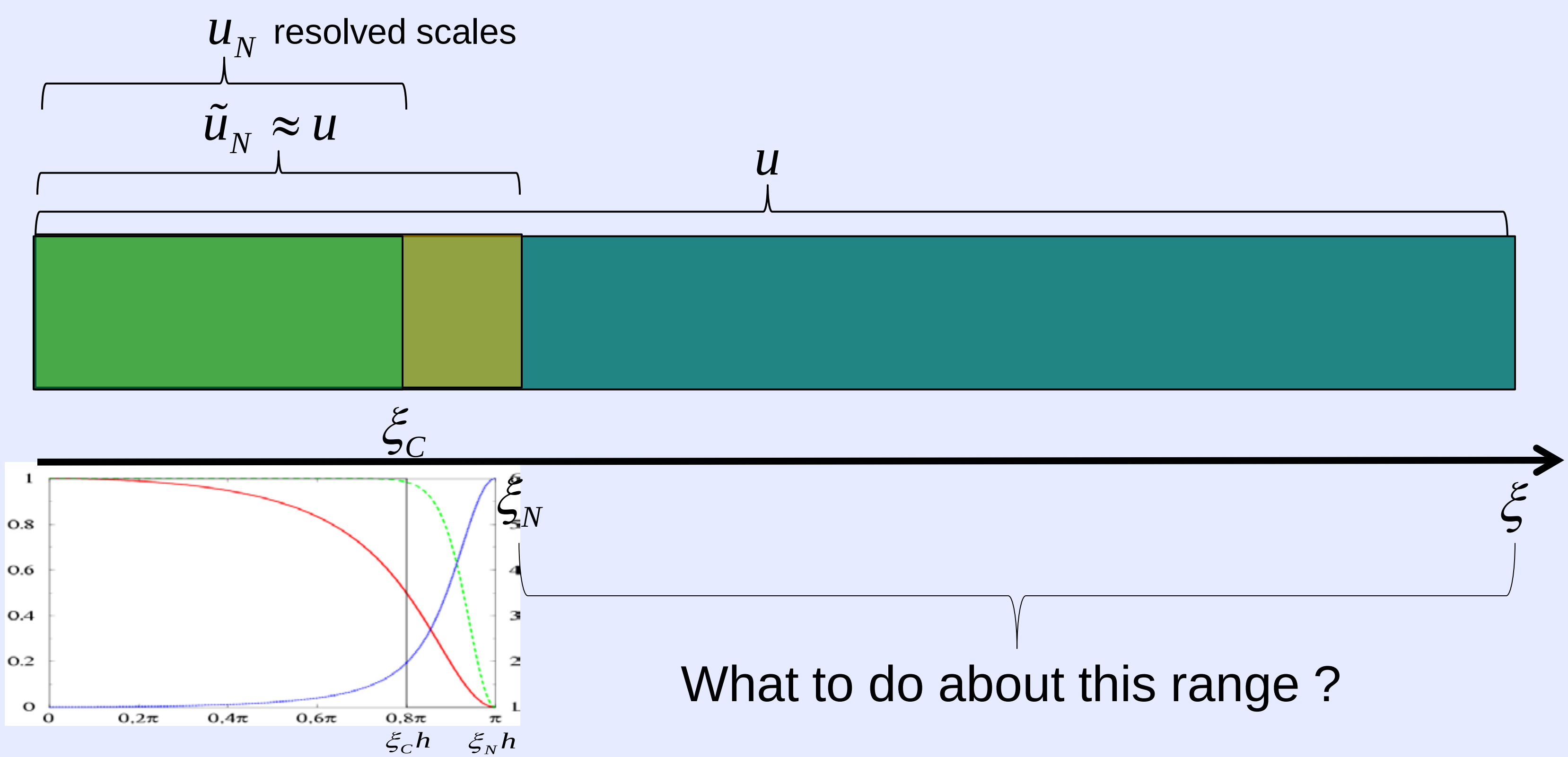
- Van Cittert regularization

$$Q = G^{-1} = [I-(I-G)]^{-1} = \sum_{\nu=0}^{\infty}(I-G)^{\nu} \approx \sum_{\nu=0}^{M}(I-G)^{\nu}$$

- Transfer functions for M=5



3. Stochastic subgrid-scale estimation



- ADM Regularization
  - **Stolz, Adams, Phys. Fluids 1999 – mentioned**
  - **Stolz, Adams, Kleiser, Phys. Fluids 2001 – done**
  - **Successfully applied as “stand-alone” model by Kleiser et al. since**

$$\frac{\partial \tau_{ij}^{(2)}}{\partial x_j} = -\chi \left(I - Q * G \right) * \overline{u}_i^N$$

3. Stochastic subgrid-scale estimation

- What is special about ADM Regularization

Quote Alan Wray (NASA Ames) about 1998:

“Oh yes, this is just a Langevin term”

(I did not pay sufficient attention to this at that time)

- Analogy between filtering and kernel estimation

Average using PDF:

$$\bar{u}_i = \int_{-\infty}^{\infty} f_{u_i}(v_i) v_i dv_i.$$

Estimator function from particles:

$$\bar{u}_i(\mathbf{x}) = \frac{\sum_\alpha G(\mathbf{x}-\mathbf{x}_\alpha) u_i(\mathbf{x}_\alpha)}{\sum_\beta G(\mathbf{x}-\mathbf{x}_\beta)}.$$

Filter as kernel estimator:

$$\bar{u}_i(\mathbf{x}) = \int_{-\infty}^{\infty} G(\mathbf{x}-\mathbf{x}'; h) u_i(\mathbf{x}') d\mathbf{x}',$$

3. Stochastic subgrid-scale estimation

- Analogy between ADM-relaxation and Pope's Generalized Langevin Model (deterministic version):

GLM-deterministic, Lagrangian

$$dw_i^\alpha = -\frac{1}{\bar\rho}\frac{\partial \bar p}{\partial x^\alpha}dt + \frac{\partial \bar\sigma^{\alpha\beta}}{\partial x^\beta}dt - \chi^{\alpha\beta}(w_i^\beta - \bar w_i^\beta)dt.$$

GLM-deterministic, Eulerian

$$\frac{\partial w^\alpha}{\partial t} + w^\beta \frac{\partial w^\alpha}{\partial x^\beta} = -\frac{1}{\bar\rho}\frac{\partial \bar p}{\partial x^\alpha} + \frac{\partial \bar\sigma^{\alpha\beta}}{\partial x^\beta} - \chi^{\alpha\beta}(w^\beta - \bar w^\beta).$$

Deterministic flow map

ADM-relaxation

$$\frac{\partial \bar u^\alpha}{\partial t} + \overline{u^{*\beta}\frac{\partial u^{*\alpha}}{\partial x^\beta}} = -\frac{1}{\bar\rho}\frac{\partial \bar p}{\partial x^\alpha} + \frac{\partial \bar\sigma^{\alpha\beta}}{\partial x^\beta} - \chi(\bar u^\alpha - \overline{u^{*\alpha}}),$$

3. Stochastic subgrid-scale estimation

- What about the full GLM ?

$$dw_i^\alpha = -\bar{F}_i^\alpha dt - F_{P_i}^\alpha dt - \chi^{\alpha\beta}(w_i^\beta - \bar{w}_i^\beta)dt + \boxed{\sqrt{\gamma}\xi_i^\alpha dt,}$$

Stochastic force $\Rightarrow$
no flow map

- Eulerian representation of Lagrangian-particle distribution by stochastic number-density field

Soulard, Sabelnikov, Combust., Explos. Shock Waves, 2006

$$\frac{\partial n}{\partial t} = -\frac{\partial}{\partial x^\alpha}\sum_i \delta(\mathbf{x}-\mathbf{x}_i)w_i^\alpha, \xrightarrow[\text{calculus}]{\text{Delta-function}} \frac{\partial n}{\partial t} + \frac{\partial m^\alpha}{\partial x^\alpha} = 0,$$

Nakamura, Yoshimori, J. Phys. A, 2009

3. Stochastic subgrid-scale estimation

- More delta-function calculus $\Rightarrow$ Eulerian GLM

Adams, Phys. Fluids, 2011

The trick

$$\frac{\partial m^\alpha}{\partial t} + \frac{\partial}{\partial x^\beta}\frac{m^\alpha m^\beta}{n} = -\bar{F}^\alpha(\mathbf{x},t)n(\mathbf{x},t) \boxed{-\frac{\partial p_s}{\partial x^\alpha}}$$
$$- \chi^{\alpha\beta}\left(m^\beta(\mathbf{x},t) - \bar{w}^\beta(\mathbf{x},t)n(\mathbf{x},t)\right)$$
$$+ \sqrt{\gamma}n(\mathbf{x},t)\zeta^\alpha(\mathbf{x},t),$$

- Stochastic extension of ADM

Adams, Phys. Fluids, 2011

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \overline{\rho u^\alpha}}{\partial x^\alpha} = 0, \tag{21a}$$

$$\frac{\partial \overline{\rho u^\alpha}}{\partial t} + \frac{\partial}{\partial x^\beta}\frac{\overline{(\rho u^\alpha)^*(\rho u^\beta)^*}}{\bar{\rho}} = -\frac{\partial \overline{p^*}}{\partial x^\alpha} - \frac{\partial \overline{\sigma^{*\alpha\beta}}}{\partial x^\beta}, \tag{21b}$$

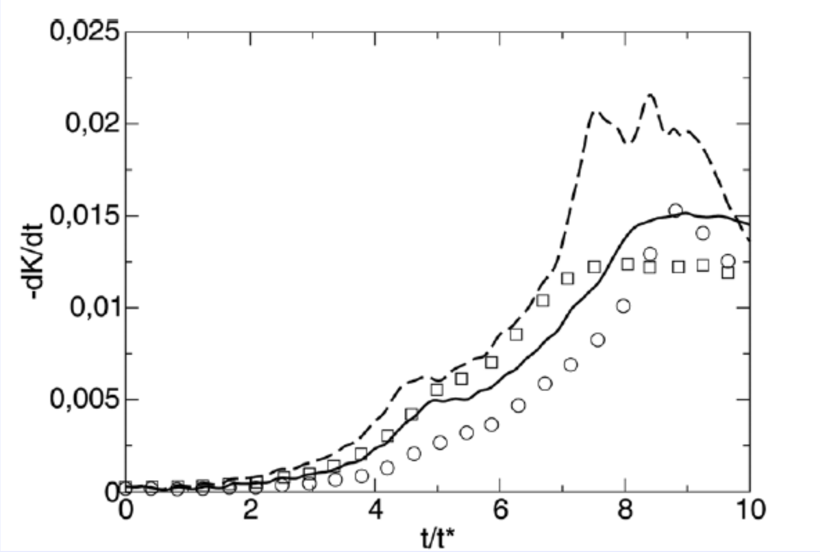
$$\frac{\partial \bar{E}}{\partial t} + \frac{\partial}{\partial x^\beta}\overline{(E^* + p^*)\frac{(\rho u^\alpha)^*}{\bar{\rho}}} = \frac{\partial}{\partial x^\beta}\overline{\sigma^{*\alpha\beta}\frac{(\rho u^\alpha)^*}{\bar{\rho}}} + \frac{\partial}{\partial x^\beta}\overline{q^{*\beta}}. \tag{21c}$$

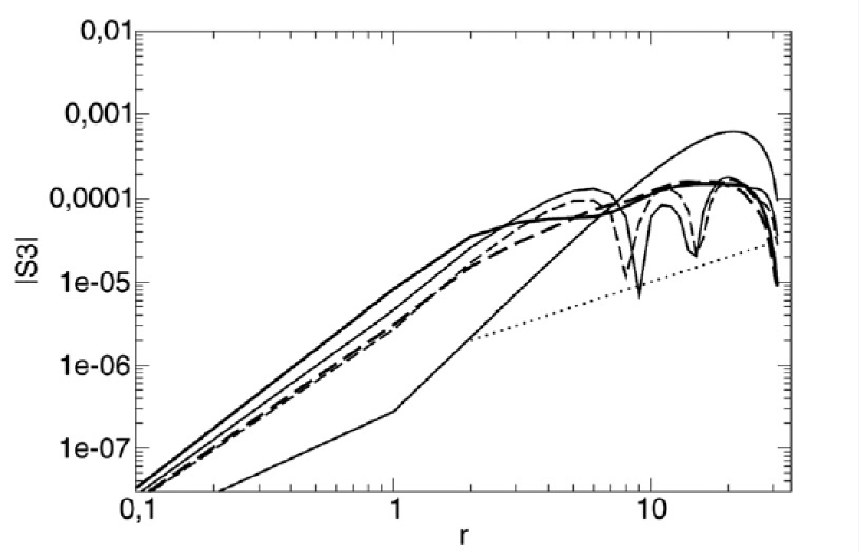
3. Stochastic subgrid-scale estimation

- Stochastic extension of ADM (continued)

$$(\rho u^{\alpha})^{*} = \overset{\overset{Q*G}{\downarrow}}{G_2} * (\overline{\rho u^{\alpha}}) + \bar{\rho}(I - \overset{\overset{Q*G}{\downarrow}}{G_2}) * \left(\frac{m^{\alpha}}{n}\right).$$

- SADM in operation (3D TGV)





Some bold statements at the end

- Physically consistent implicit LES is probably the final development of *numerical* LES and will be the main tool for future practical applications

- A large grey zone will develop / develops with marginally physically consistent implicit LES approaches

- Meso-scale modeling and simulation with theoretically rather well established stochastic meso-scale (subgrid-scale) models is an emerging field for many fluid-mechanics applications