Large-Eddy Simulation: state-of-the-art
(with emphasis on multiscale methods)

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GTP Workshop « LES of MHD turbulence »

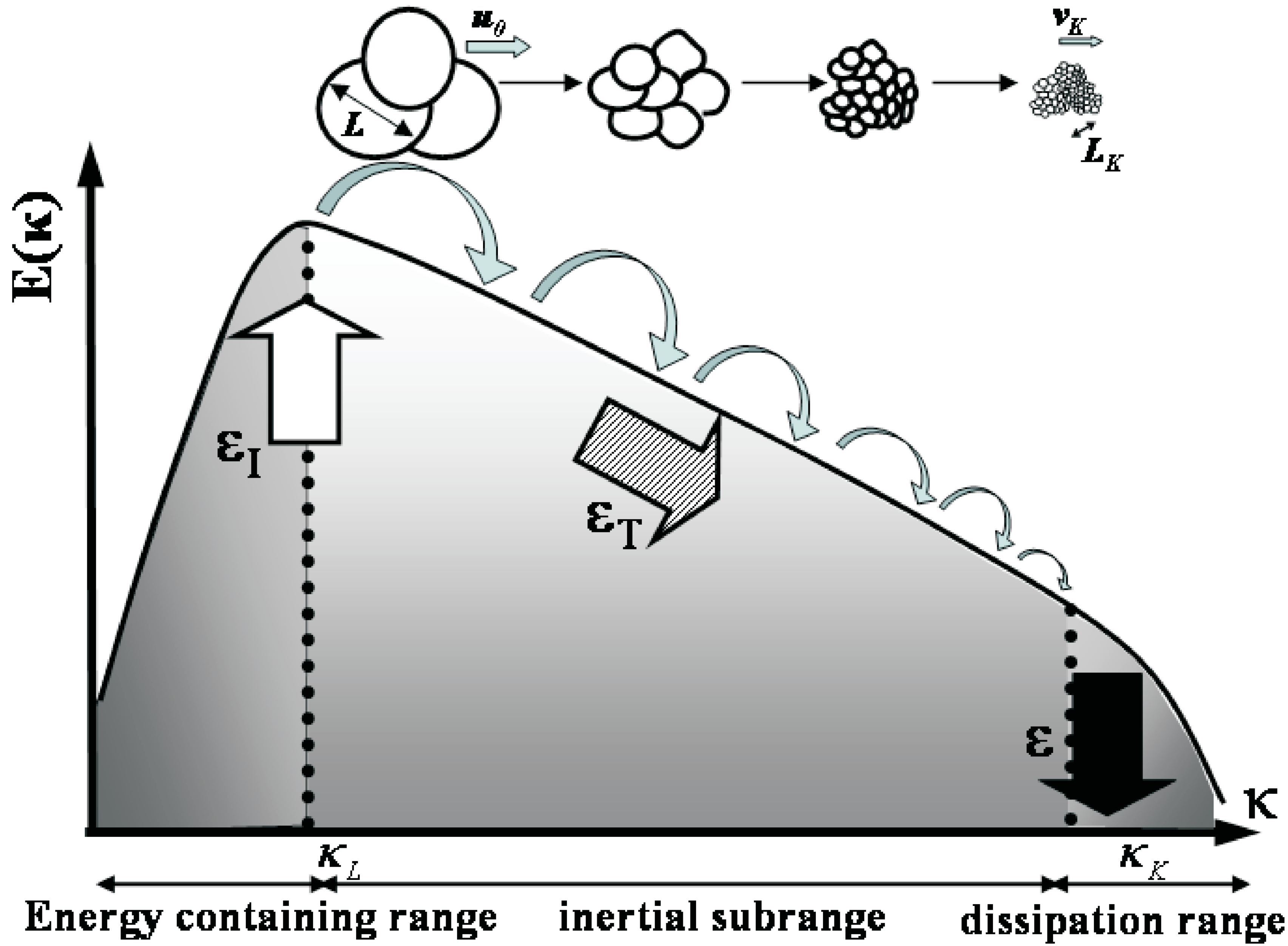
NCAR, Boulder, Colorado

20-23 May, 2013

Outline

1. Turbulence as a multiscale phenomenon: a brief reminder
2. Capturing turbulence features: grid resolution, scale separation
3. Multiscale/adaptive grid DNS/LES methods: a survey
4. Some open issues

Turbulence dynamics: Kinetic energy cascade



2. Grid resolution & scale separation

Is Direct Numerical Simulation possible ?

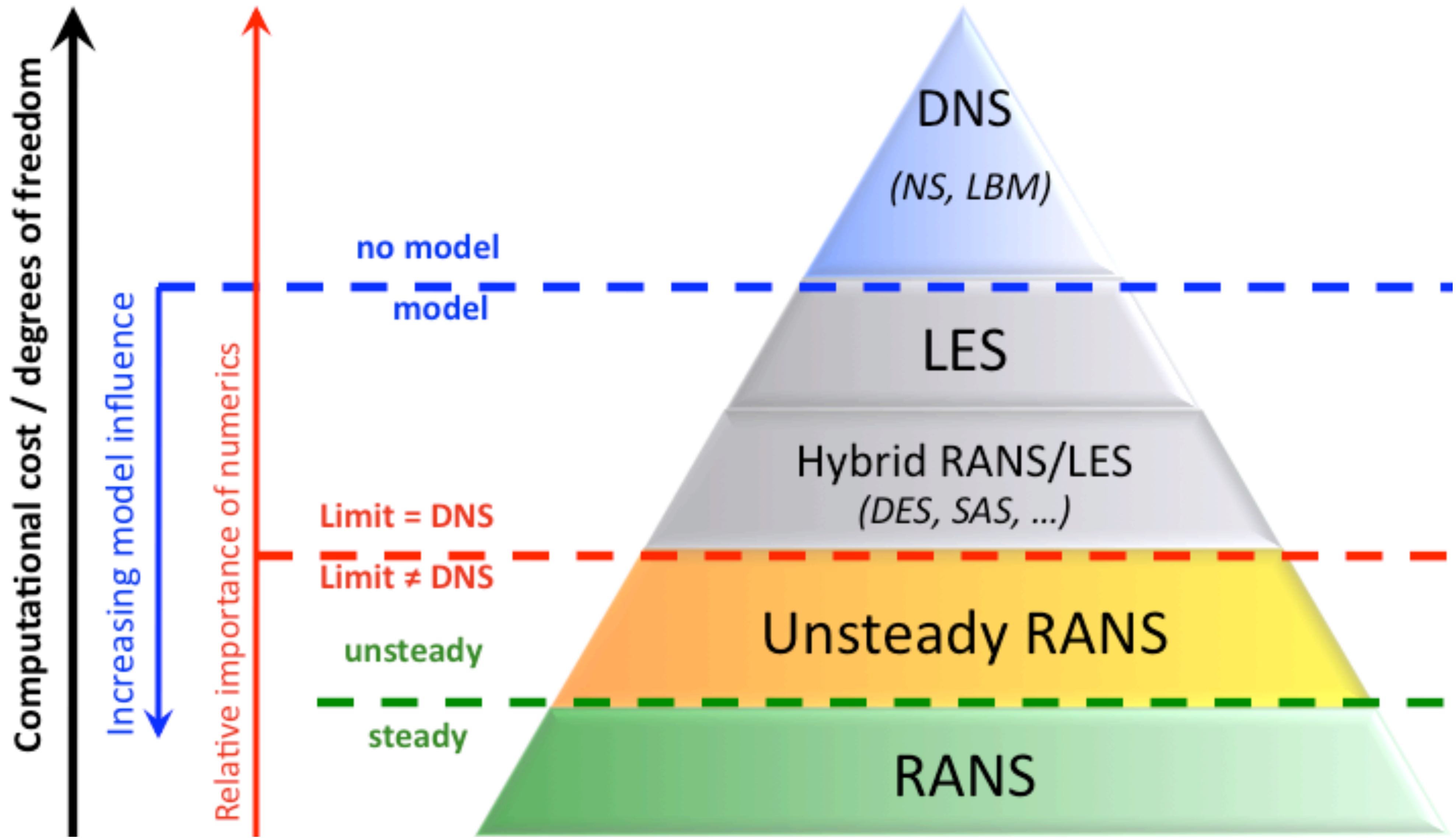
Number of grid points: $$\left(\frac{Lx}{\Delta x}\right)^3 \sim \left(\frac{L}{\eta}\right)^3 \sim (Re_L^{3/4})^3 \sim Re_L^{9/4}$$

Number of time steps: $$\left(\frac{T}{\Delta t}\right) \sim \left(\frac{L_T}{\tau_\eta}\right) \sim Re_L^{1/2}$$

Total complexity: $$Re_L^{1/2} \times Re_L^{9/4} = Re_L^{11/4}$$

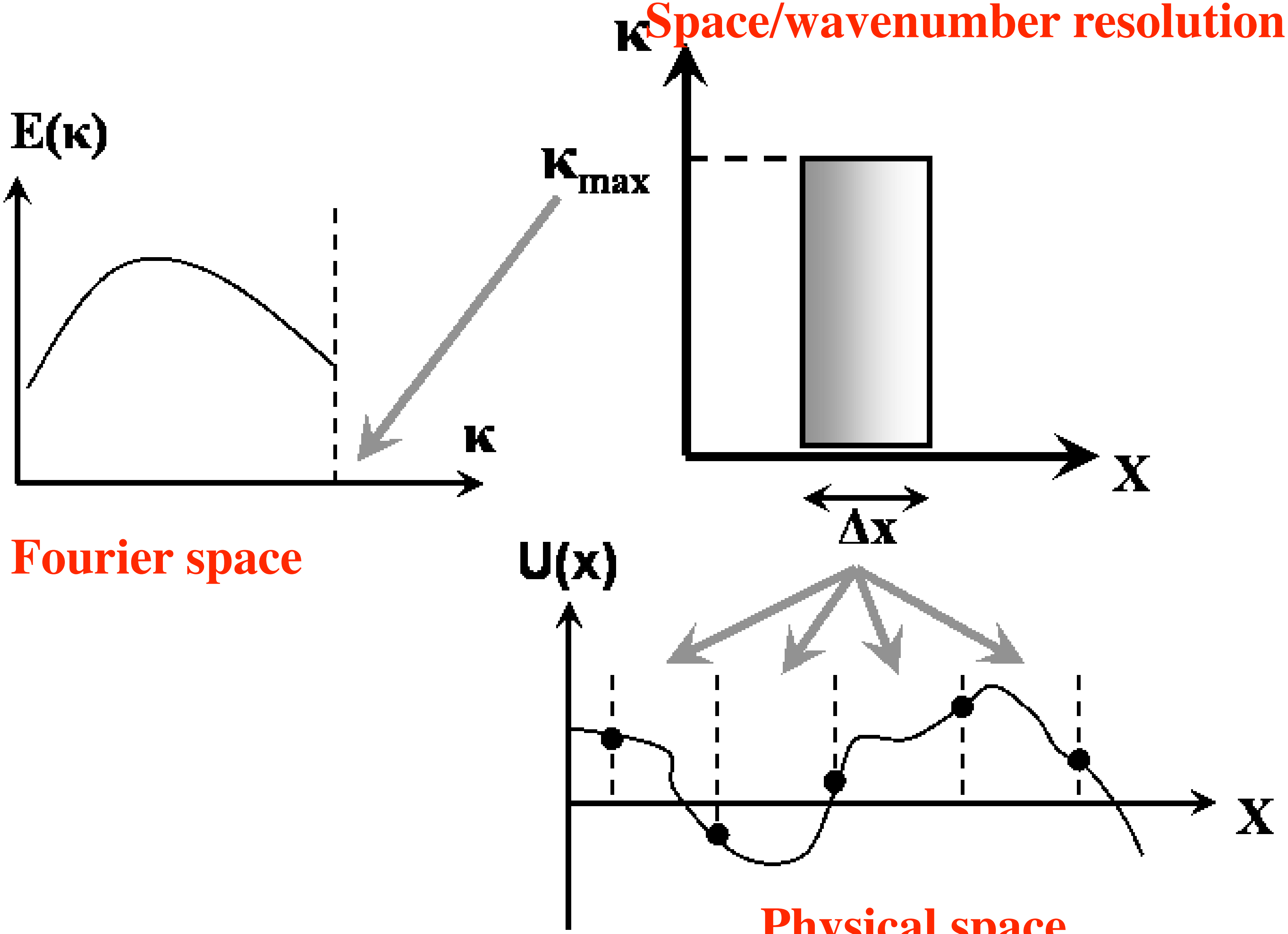
Hierarchy of CFD methods

*« **Multiscale & Multiresolution approaches for turbulence, 2nd edn** »*
Sagaut, Deck & Terracol, Imperial College Press, 2013



Small scale removal

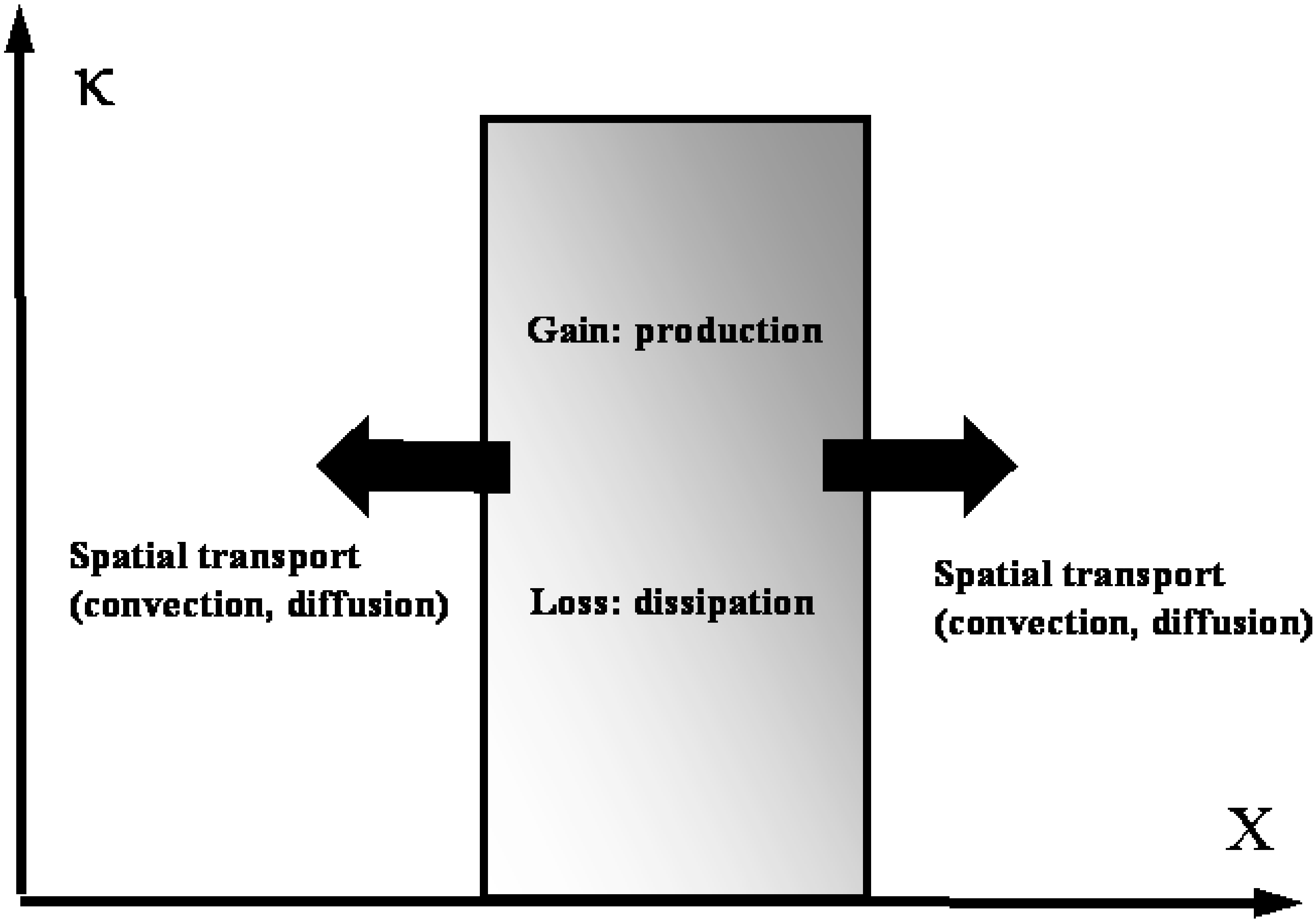
Space/wavenumber resolution



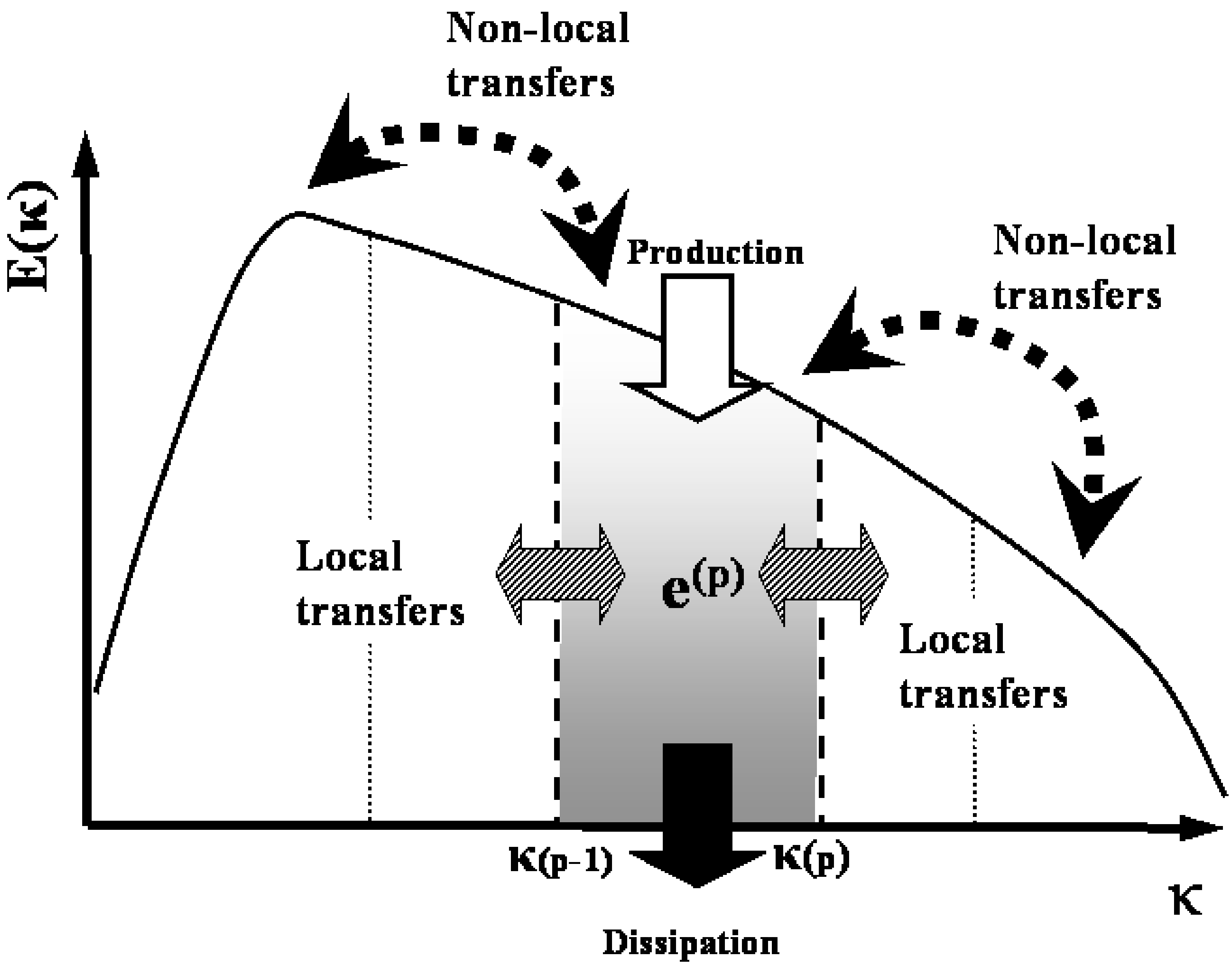
Fourier space

Physical space

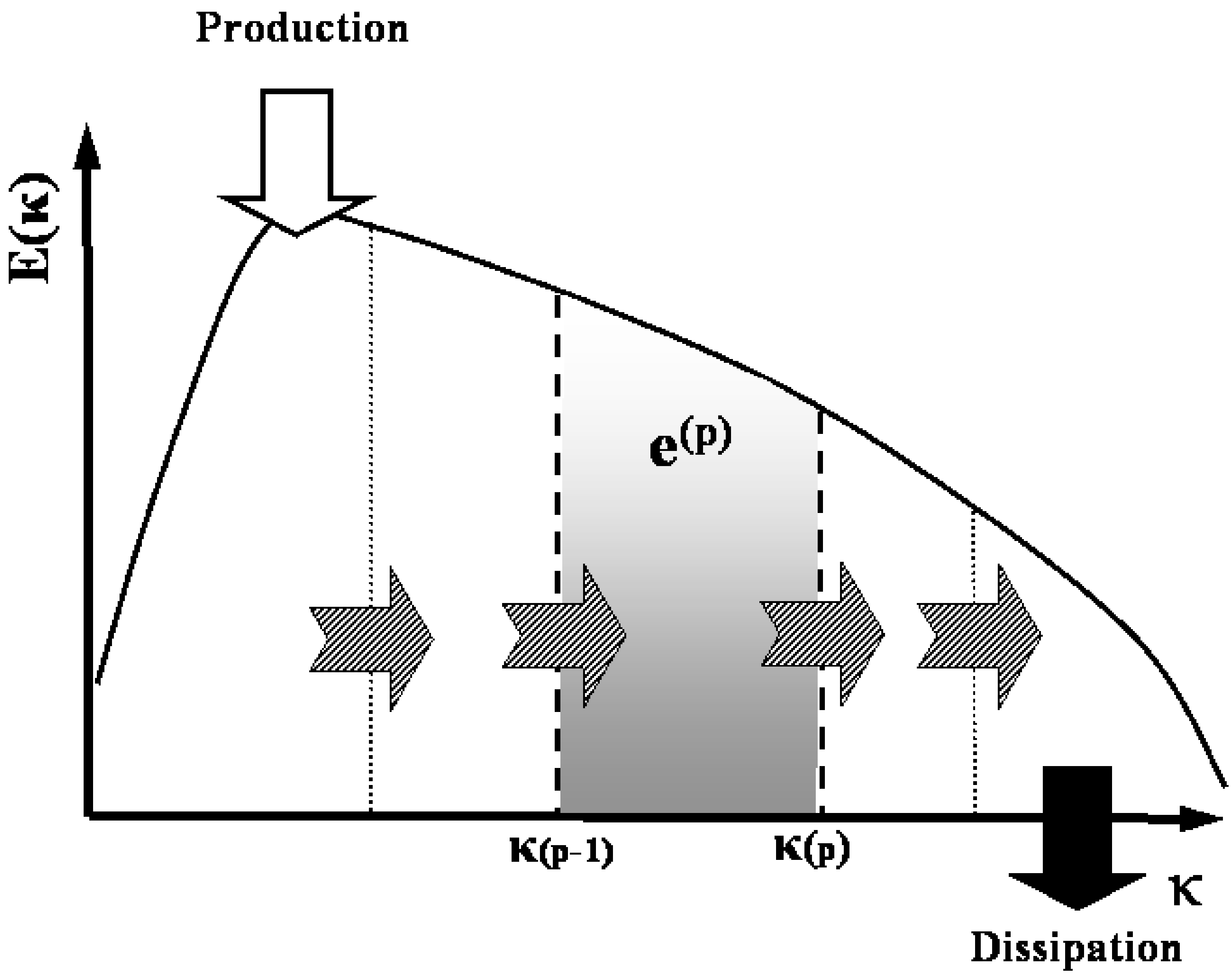
Control cell energy budget: physical space



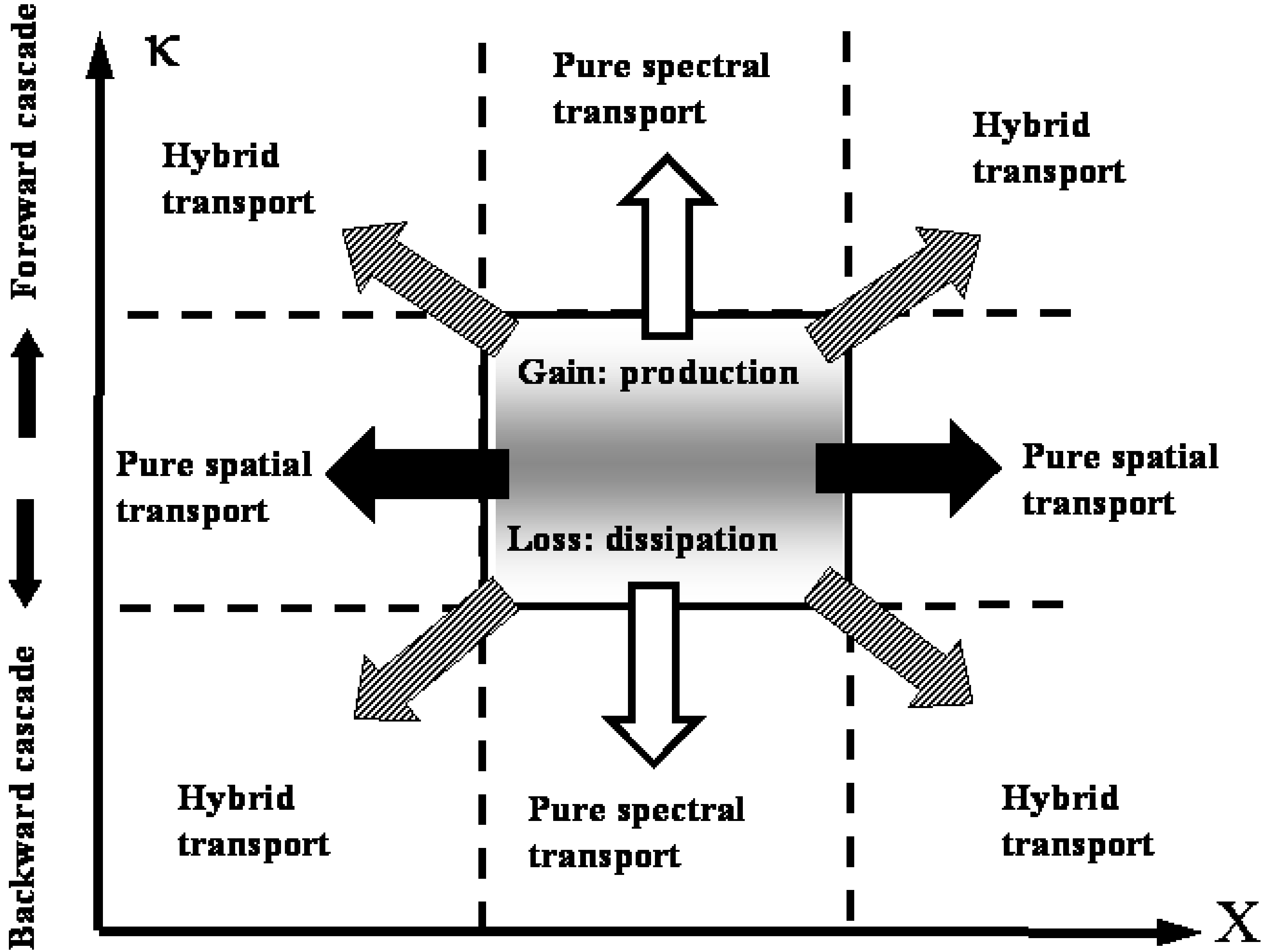
Control cell energy budget: Fourier space



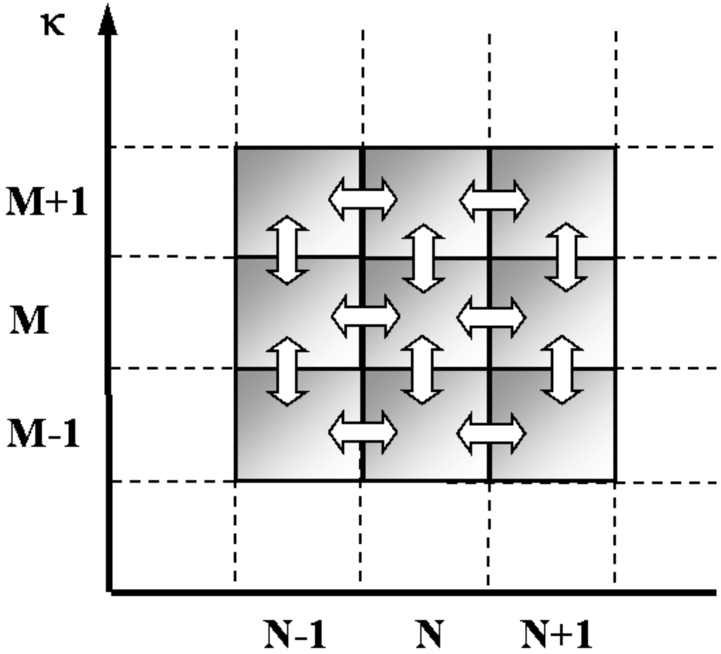
Simplified view: schematic direct cascade



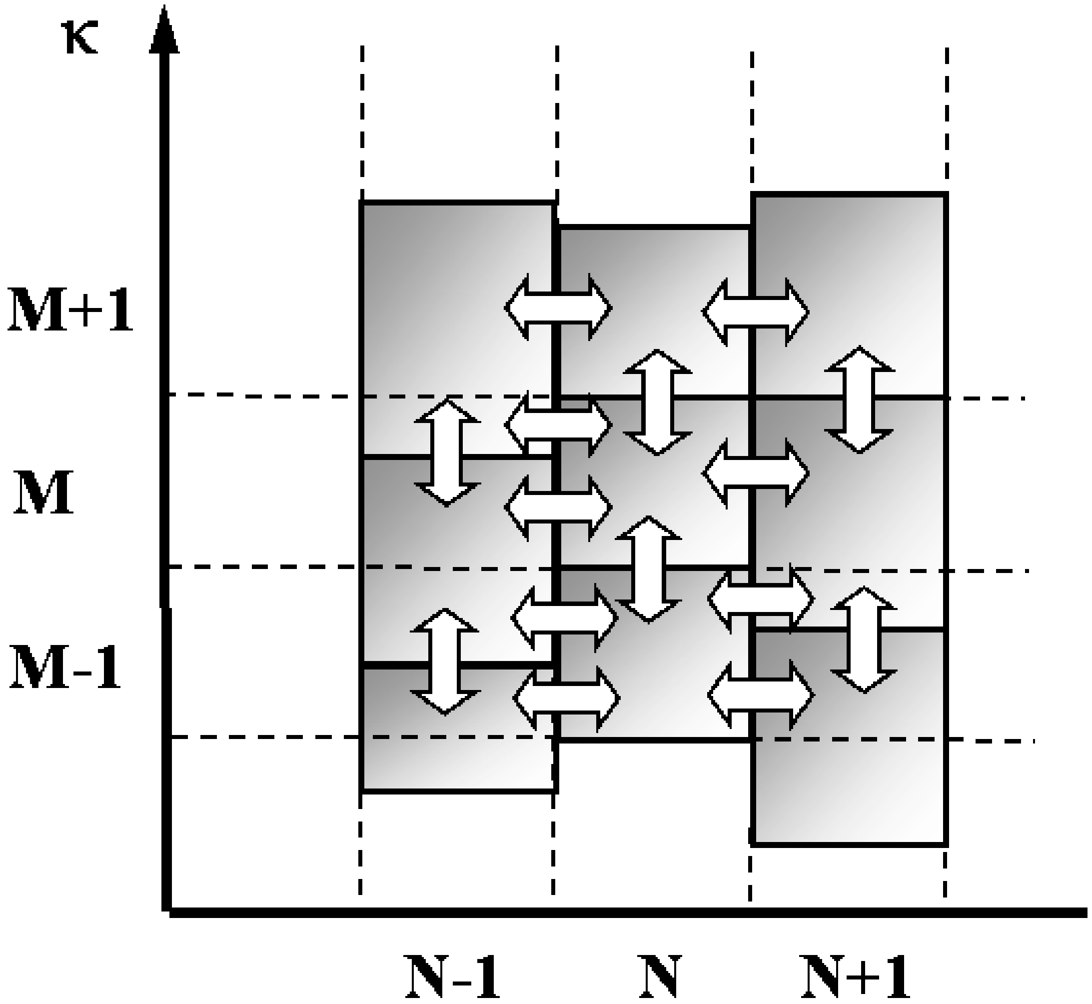
Physical/Fourier space energy budget



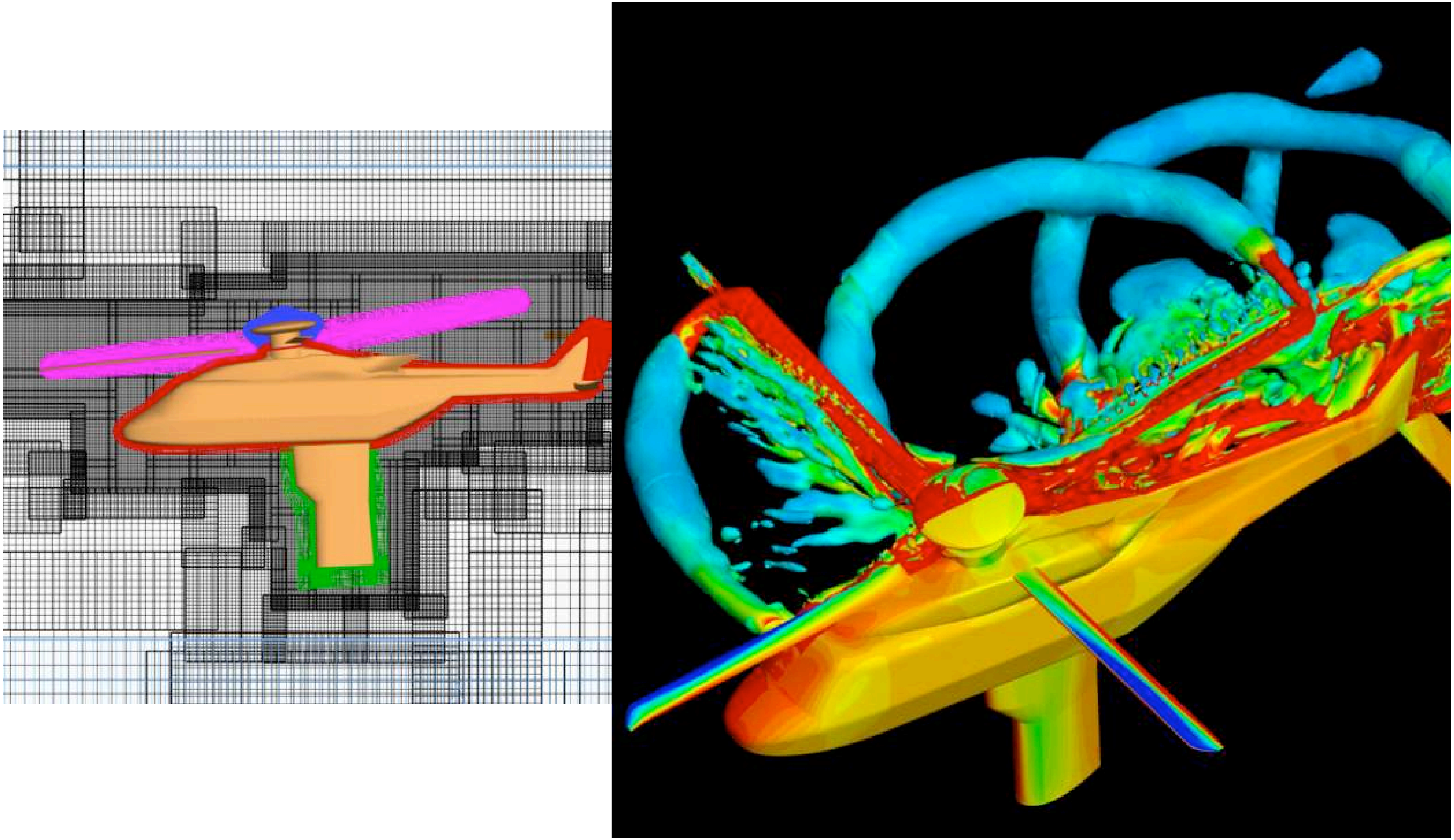
Conformal/non-conformal mapping



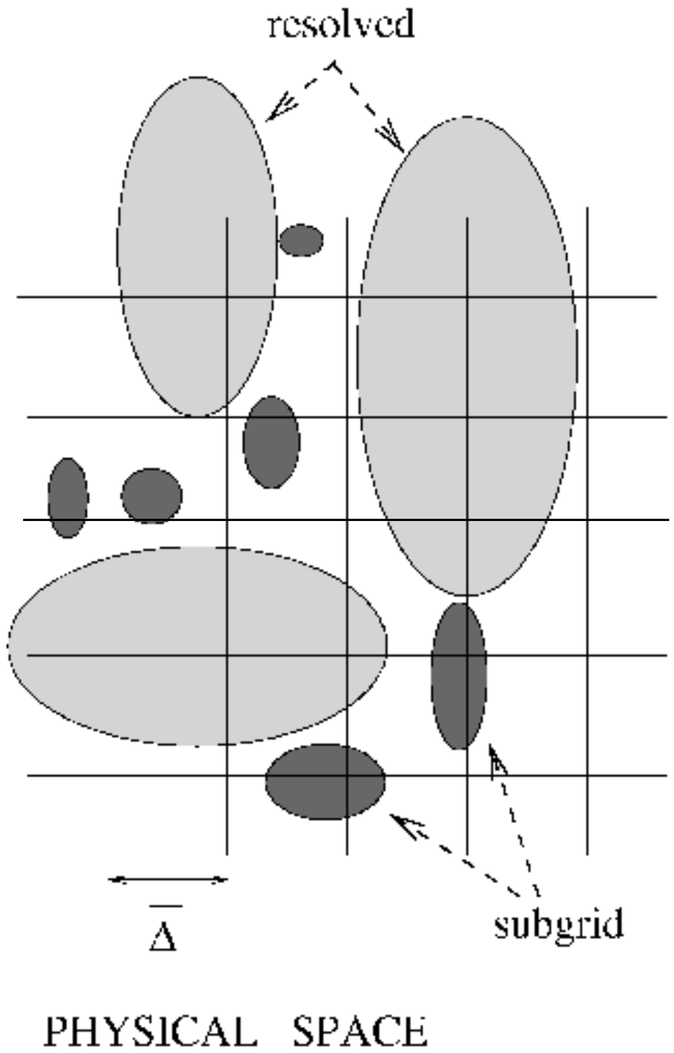
Non-conformal spectral mapping

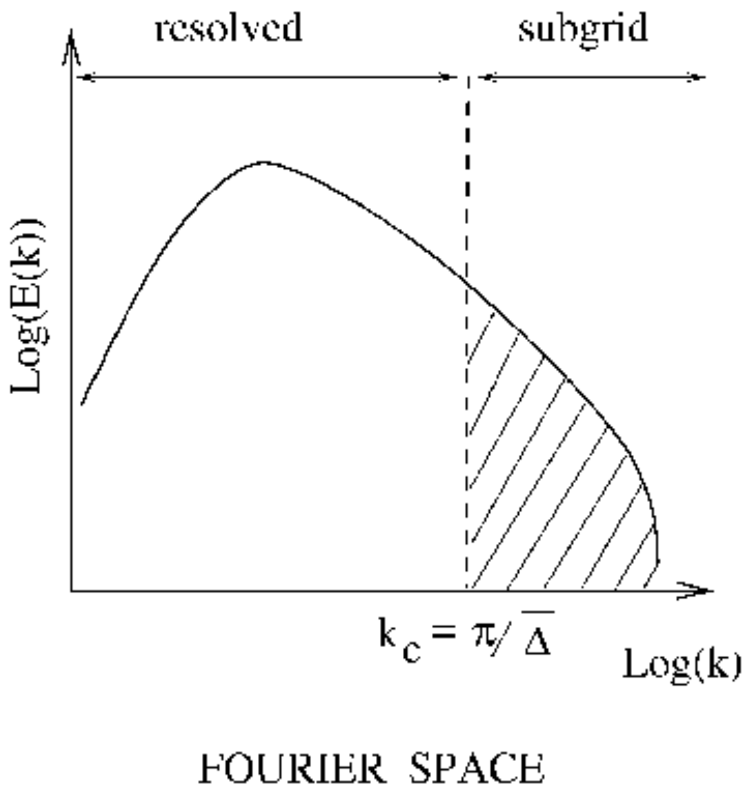


Multiscale/adaptive grid DNS/LES methods



LES: the key observation





LES: a deeper analysis

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

u: exact turbulent solution

$$\frac{\delta u_h}{\delta t} + F_h(u_h,u_h) = 0$$

u_h: discrete solution

LES:

- discrete solution ➪ **projection error**
- approximate integro-differential operators ➪ **discretization error**
- unresolved scales ➪ **resolution error**

LES : Modified PDE Model

Discrete numerical model

$$\frac{\delta u_h}{\delta t} + F_h(u_h, u_h) = 0$$

Equivalent continuous PDE

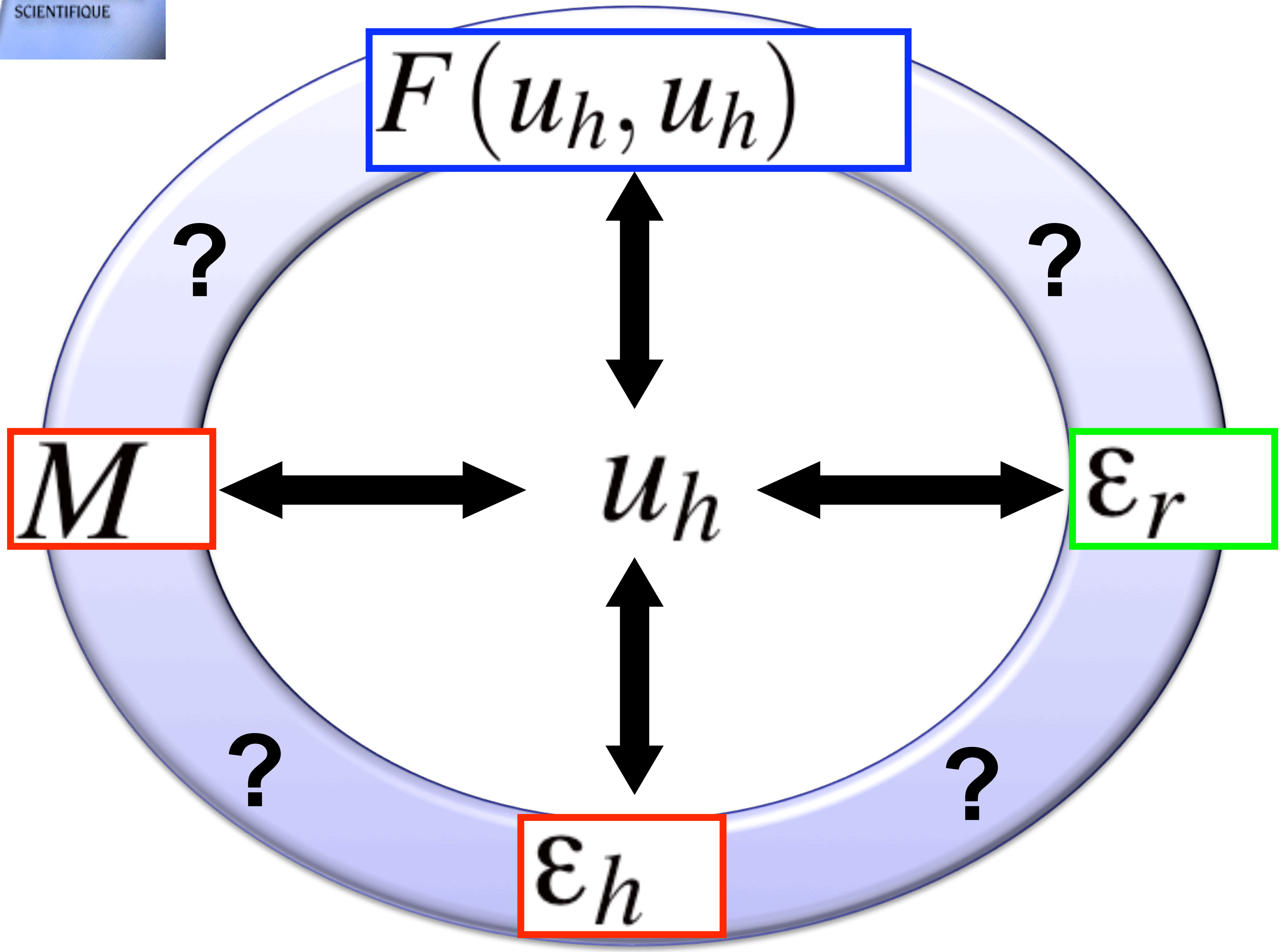
$$\frac{\partial u_h}{\partial t} + F(u_h, u_h) = M + \varepsilon_r + \varepsilon_h$$

Exact subgrid model

numerical error

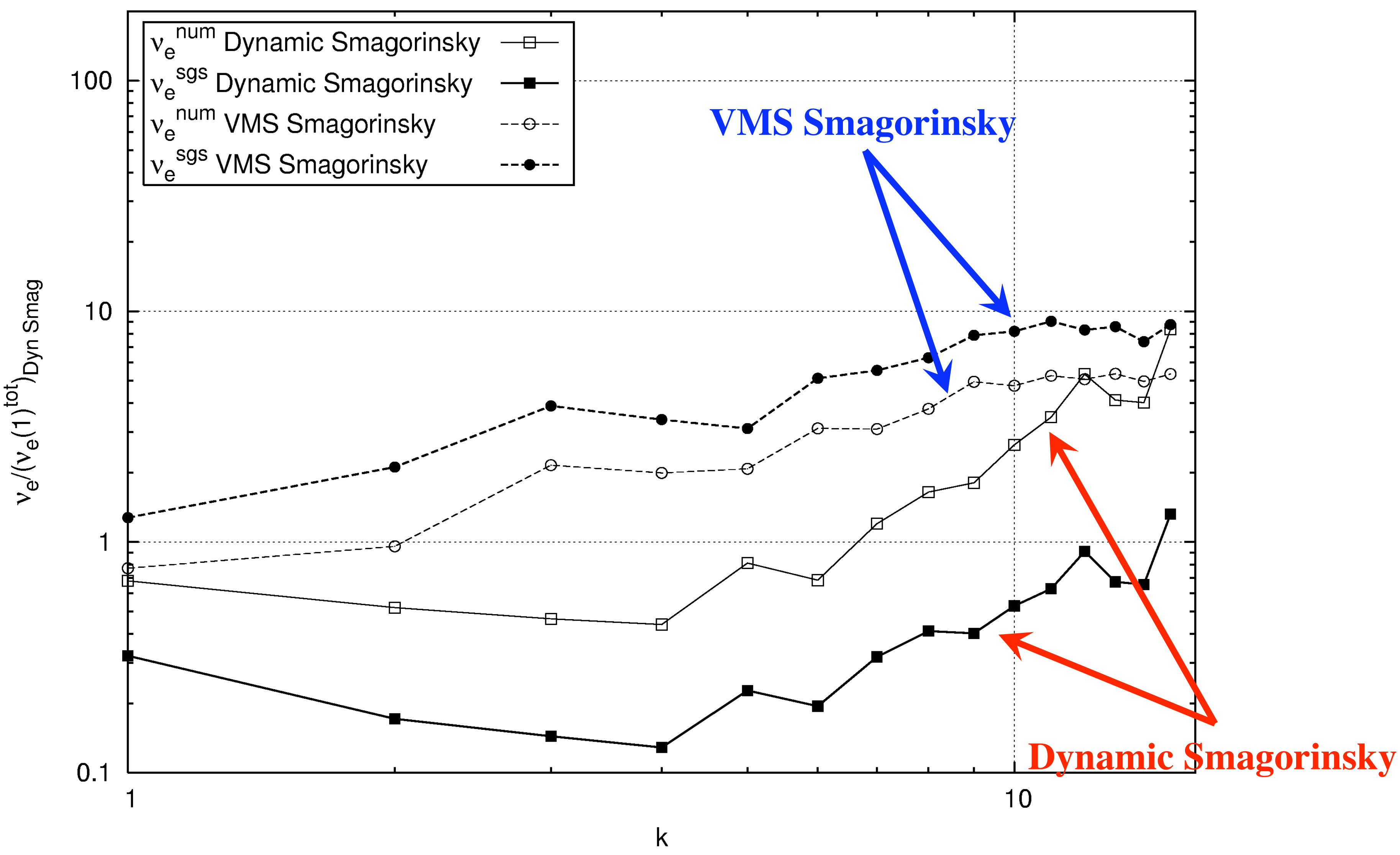
Subgrid modelling error

Implicit non-linear couplings in LES



E.g. Numerical and VMS viscosities

(Ciardi & al., JOT, 2006)



Definition of the optimal LES solution

$$\min(e_\pi + e_h + e_r) = \min(e_\pi)$$

$$e_h + e_r = 0$$

Implicit LES:

- No physical subgrid model
- Ad hoc scheme

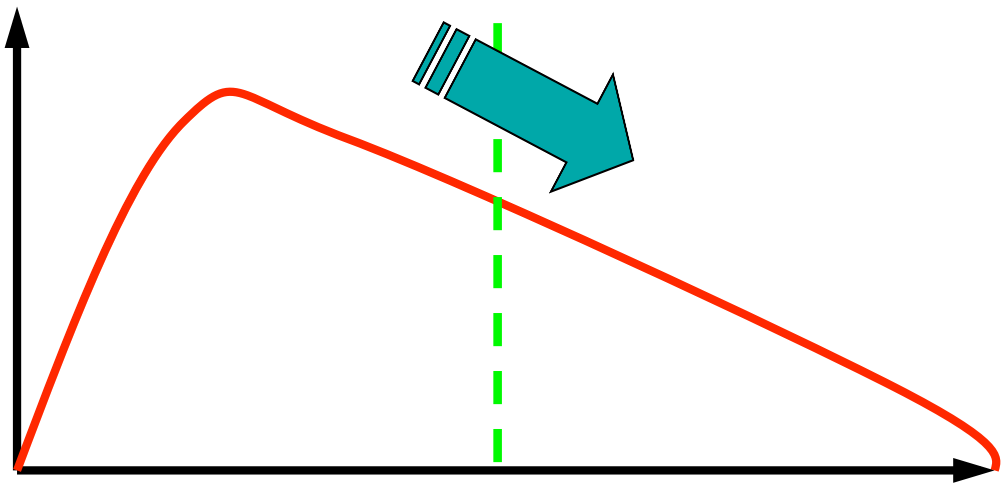
$$e_h = e_r = 0$$

Classical LES:

- Explicit subgrid model
- Neutral scheme

Functional models:

– Surrogate for the mean interaction
– ***Hyp 1***: Kinetic energy balance is most important
– ***Hyp 2***: TKE cascade is dominant→ dissipative action in the mean



– ***Hyp 3***: An eddy-viscosity model is relevant

If there is something more occuring, this is not a small/subgrid scale !

A priori constraints for subgrid models

- Consistency (1) : subgrid model should vanish in fully resolved regions
- Consistency (2) : some subgrid scale effects must be recovered (e.g. net kinetic energy transfer associated with kinetic energy cascade)
- Consistency (3) : symmetries of the exact LES equations must be preserved
- Subgrid models must be 'user friendly'

Smagorinsky model (1963)

- Subgrid tensor model:

$$S \simeq -2\nu_t \mathcal{S} \qquad \mathcal{S} = \frac{1}{2}(\nabla\bar{u} + \nabla^T\bar{u})$$

- Subgrid viscosity model

$$\nu_t = (C_S\Delta)^2|\mathcal{S}|$$

Arbitrary constant

Cutoff length scale

Cont'd

- Remarks:
  - Reminiscent of von Neumann - Richtmyer artificial viscosity for shock capturing (1950)
  - Belongs to Ladyzenskaja's class of viscosity
- Subgrid model constant must be tuned to enforce the desired rate of kinetic energy dissipation

The Smagorinsky Constant

- Canonical analysis:
  - Infinite inertial range

$$E(k) = K_0 \varepsilon^{2/3} k^{-5/3}$$

  - Local equilibrium: production = dissipation

➩« Universal value »:

$$C_S = \frac{1}{\pi}\left(\frac{3K_0}{2}\right)^{-3/4} \simeq 0.18$$

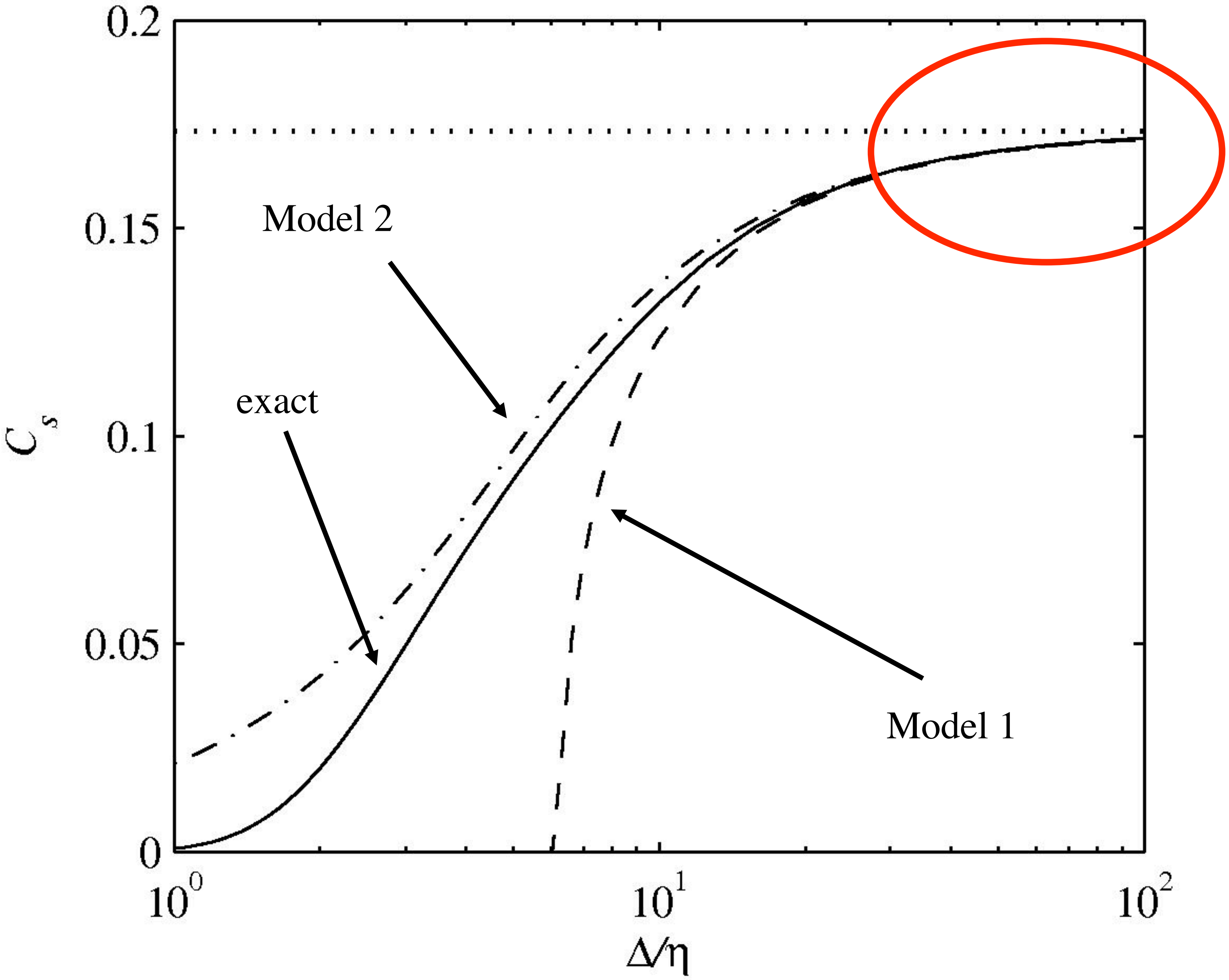
Accuracy in isotropic turbulence

- Satisfactory recovery of E(k) at infinite Reynolds number (non-dissipative numerical method, cutoff within inertial range)
- Not coherent with realistic TKE spectrum, i.e. does not account for

$$L/\Delta \quad \text{and} \quad \eta/\Delta$$

➪ 'Smagorinsky constant' not constant !

Slow asymptotic convergence !



Remark

- Usual asymptotic value C=0.18 valid if

$$L/\Delta > 10 \quad \text{and} \quad \Delta/\eta > 100$$

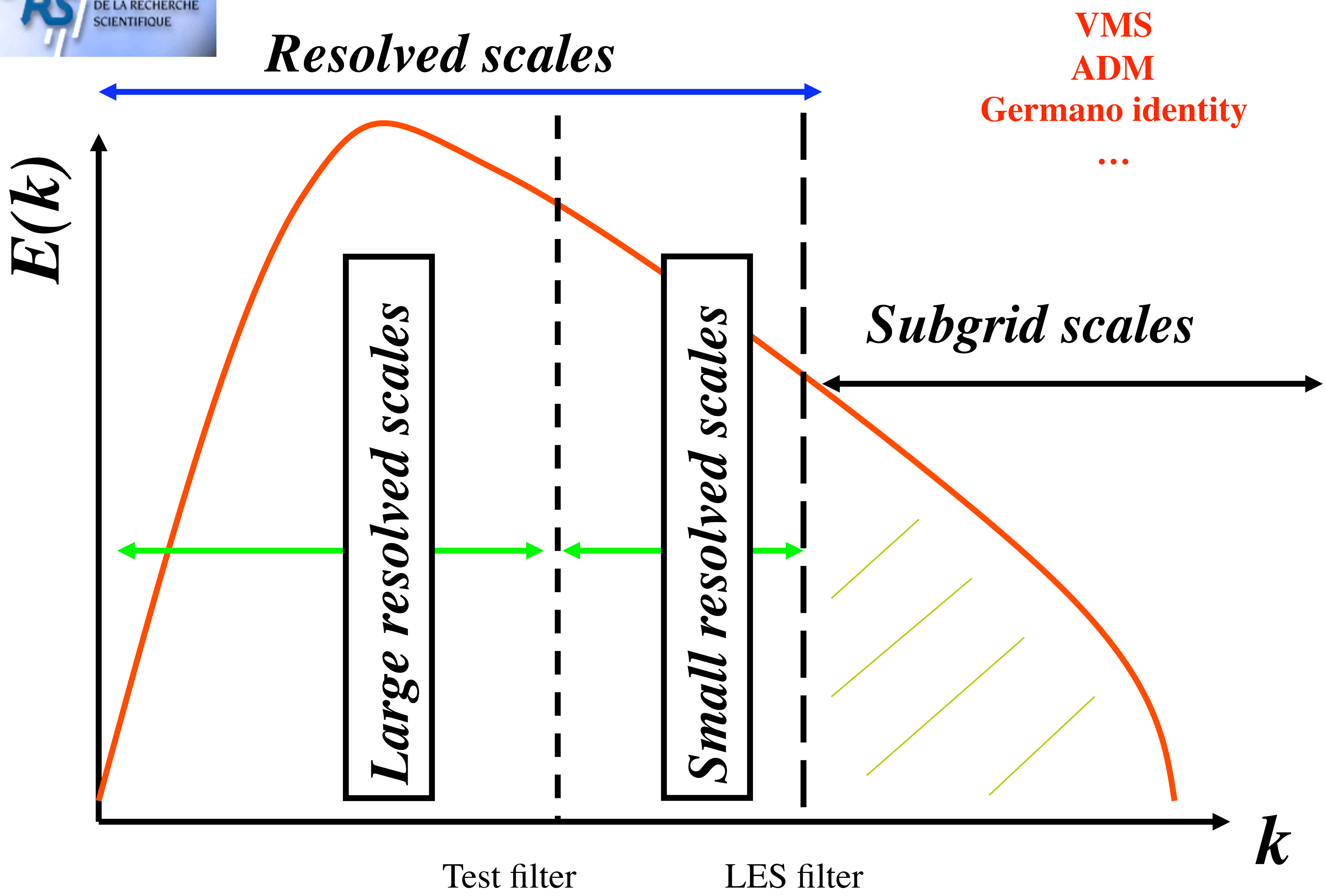
therefore

$$L/\eta > 1000 \Longrightarrow Re_L > 10^4$$

More general/self-adpative subgrid models

- ***Local automatic tuning of C_S***
  - Germano's identity ➪ least square optimization
  - Kolmogorov equation ➪ dissipation optimization *(Shao et al.)*
- ***Improved localness in terms of wave number***
  - Variational Multiscale methods
  - Filtered models
- Remark: all these approaches are based on a ***test filter***
  - The resolved field is decomposed into spectral bands
  - Features of turbulence are used/extrapolated to calibrate the subgrid models

Schematic view of test filtering



2-level Dynamic Models

Key idea: least-squre optimization of SGS model constant using the (exact) Germano identity

$$\underbrace{\widetilde{\bar{u}\bar{u}} - \tilde{\bar{u}}\tilde{\bar{u}}}_{L} = \underbrace{\widetilde{\overline{uu}} - \tilde{\bar{u}}\tilde{\bar{u}}}_{T} - \underbrace{\widetilde{\overline{uu} - \bar{u}\bar{u}}}_{\tilde{\tau}}$$

Subgrid modelling:

$$\tau = C_d f(\bar{u}, \bar{\Delta})$$

$$T = C_d f(\tilde{\bar{u}}, \tilde{\bar{\Delta}})$$

Dynamic Models

Residual definition

$$R = L - C_d \underbrace{\left(f(\widetilde{\bar{u}}, \widetilde{\bar{\Delta}}) - \tilde{f}(\bar{u}, \bar{\Delta}) \right)}_{M}$$

Least-square minimization:

$$\frac{\partial R^2}{\partial C_d} = 0$$

Solution:

$$C_d = \frac{L : M}{M : M}$$

Approximate Deconvolution Models

[Adams et al., Phys. Fluids, 1999, 2001]

- Key idea: find an approximate 'de-filtered' field

$$u^\star \equiv G_l^{-1}(\bar{u}) \sim u + O(\Delta^l)$$

- Remarks
  - Developed using the convolution filter model
  - No underlying assumption on flow physics
  - Issue: how to find the adequate approximate inverse if the exact filtering operator is not known ?

Cont'd

- ADM momentum equation

$$\frac{\partial \bar{u}}{\partial t} + \nabla.(\overline{u^\star u^\star}) + \nabla \bar{p} - \nu \nabla^2 \bar{u} = \underbrace{-\chi(I - G_l^{-1} \circ G)\bar{u}}$$

Non linear term computed using the surrogate field: does not account for u'

Dissipative regularization term used to prevent energy pile-up in resolved scales (net drain associated with kinetic energy cascade)

Implementation of the inverse filter

- ***Approximate iterative deconvolution***

$$G^{-1} = (I - (I - G))^{-1} = \sum_{p=0,+\infty} (I - G)^p$$

$$G_l^{-1} = \sum_{p=0,l} (I - G)^p$$

Truncated expansion

- Remarks
  - Known as the van Cittert deconvolution in signal processing
  - l=5 in is enough in practice *(Stolz & Adams)*
  - l=1 : Bardina's scale-similarity model
  - Obviously dependent on the evaluation of *G*
  - Can be replaced by other methods: conjugate gradient, …

Cont'd

- Approximate differential expansions

$$\bar{u}(x,t) = \int G(\Delta, |x-y|)u(y,t)dy$$

Convolution filter model

$$u(y,t) = u(x,t) + \sum_{k=1,+\infty} \frac{(y-x)^k}{k!}\frac{\partial^k u}{\partial x^k}$$

Regularity hypothesis

$$\Rightarrow \quad \bar{u}(x,t) = \left(I + \sum_{k=1,+\infty} \frac{(-1)^k}{k!}\Delta^k M_k \frac{\partial^k}{\partial x^k} \right) u$$

$$\Rightarrow \quad u(x,t) = \left(I + \sum_{k=1,+\infty} \frac{(-1)^k}{k!}\Delta^k M_k \frac{\partial^k}{\partial x^k} \right)^{-1} \bar{u}$$

Cont'd

- Usual form: *Truncated explicit Taylor series expansion*

$$u(x,t) = \left(I - \sum_{k=1,l} \alpha_k \frac{(-1)^k}{k!} \Delta^k M_k \frac{\partial^k}{\partial x^k} \right) \bar{u}$$

- Alternative forms:
  - Padé approximant
  - 'Best' polynomial projection (minimax, least-square, …)
- Remarks
  - l=2 ➪ Clark's gradient model (= tensor diffusivity model)
  - Anti-diffusion in some directions

Filtering Implementation

[Matthew et al., Phys. Fluids, 2003]

ADM can be recast as an explicit-filter-based ILES method

Exact LES eq. $$\frac{\partial \bar{u}}{\partial t} + G \star \nabla \cdot f(u) = 0$$

ADM eq. $$\frac{\partial \bar{u}}{\partial t} + G \star \nabla \cdot f(u^\star) = 0$$

$$\Rightarrow \quad G \star \left(\frac{\partial u^\star}{\partial t} + \nabla \cdot f(u^\star) \right) = G \star \frac{\partial u^\star}{\partial t} - \frac{\partial \bar{u}}{\partial t} \simeq 0$$

Cont'd

- Three-stage procedure

① $$u^{\star(n)} = G_l^{-1} \star \bar{u}^{(n)}$$

② $$u^{\star(n+1)} = u^{\star(n)} + \Delta t \frac{\partial u^\star}{\partial t}$$

③ $$\bar{u}^{(n+1)} = G \star u^{\star(n+1)}$$

Just need 1 DNS step, 1 filtering step, 1 defiltering step

Cont'd

- **Two-stage procedure** (= explicit linear filtering step in DNS code !)

① $$\hat{u}^{(n)} = \underbrace{(G \star G_l^{-1})}_{H} \star \bar{u}^{(n)}$$

② $$\bar{u}^{(n+1)} = \hat{u}^{(n)} + \Delta t \frac{\partial \hat{u}^{(n)}}{\partial t}$$

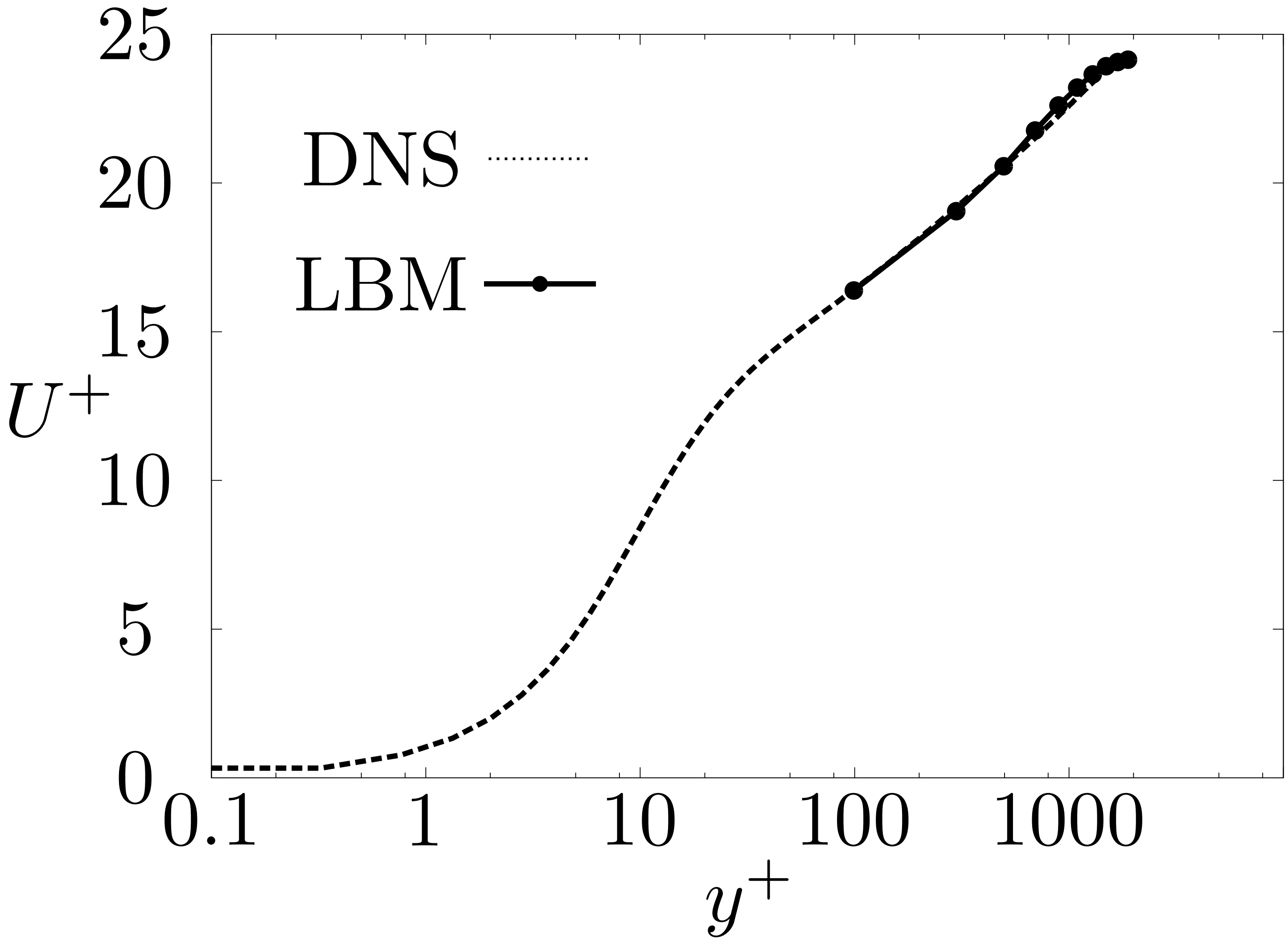
- Just need 1 DNS step, 1 filtering step

- use H^2 instead of H to account for regularization if $\chi = 1/\Delta t$

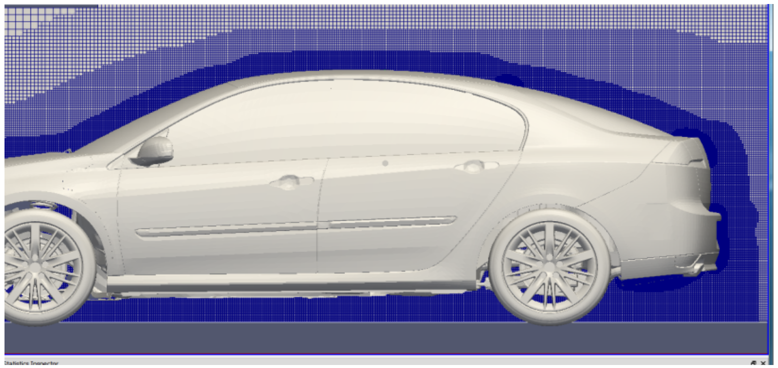
Wall Model for LBM-LES

Channel flow at $Re_\tau = 2003$

$$\Delta x^+ = \Delta y^+ = \Delta z^+ = 200$$



Validation on full-scale vehicles

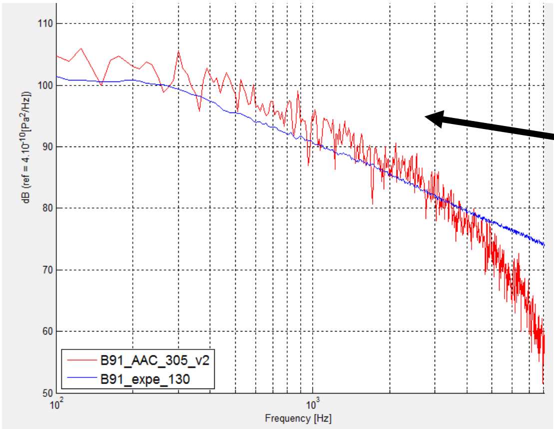


- Full scale vehicle simulation
- 186 surfaces (2,3 millions surface triangles)
- 10 levels of grid refinement, 88.6 millions cells
- dx_min=1.25mm
- 300 000 time steps → 0.96 sec
- U0 = 44.4 m/s
- Wall Model in first cell LES
- LBM-ADM model

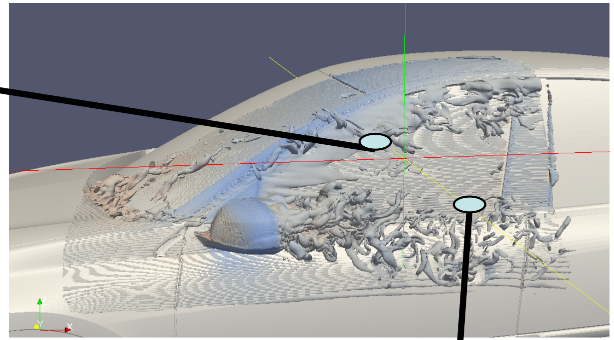
Validation on full-scale vehicles

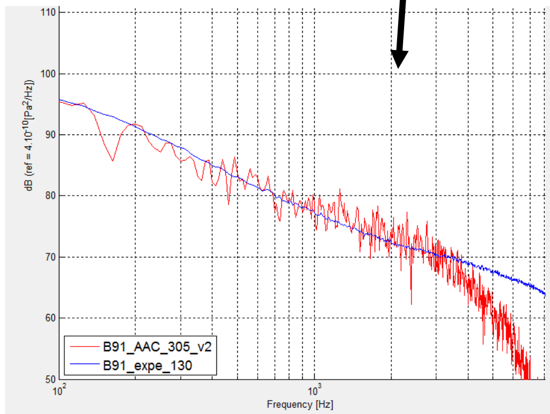
LaBS

Measurements

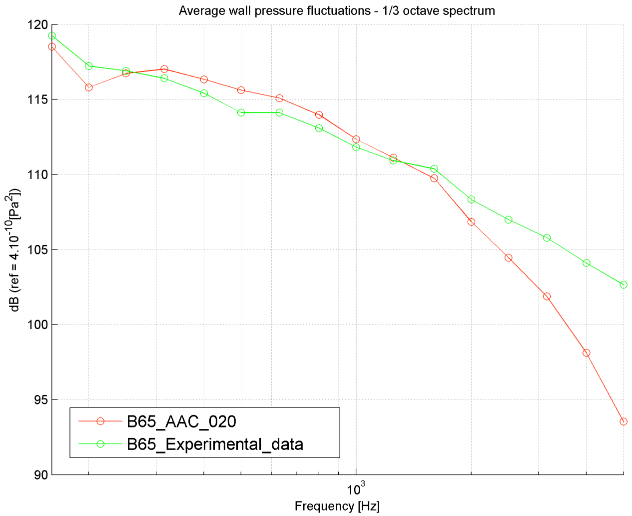


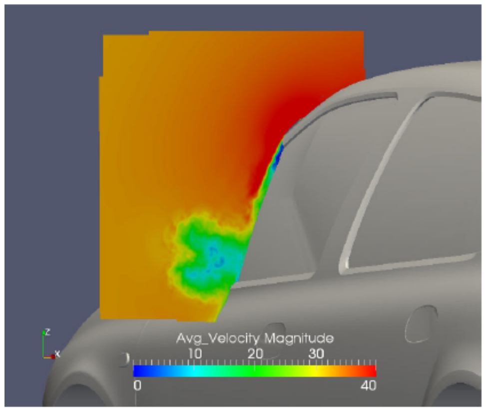
Laguna case : fine band spectra





Clio case : third-octave band spectra, averaged on the whole surface of the side window





A few comments

Classical LES for engineering applications:

• no production mechanism at subgrid scale (exception : wall models for turbulent boundary layers)

• mostly eddy viscosity models

• no account for anisotropy at small scales

• sometimes eddy-viscosity tuning for physical effects on non-linear cascade (e.g. stable stratification

• Improvement of the results: grid refinement !

A few existing AMR-LES methods

- **Terracol's multilevel LES**

[Terracol et al., JCP 167, 2001]
[Terracol et al., JCP 184, 2003]
[Terracol & Sagaut, Phys. Fluids 15(12), 2003]

- **Hoffman's Adaptive Grid DNS/LES**

http://www.csc.kth.se/~jhoffman/Johan_Hoffman_KTH/Home.html

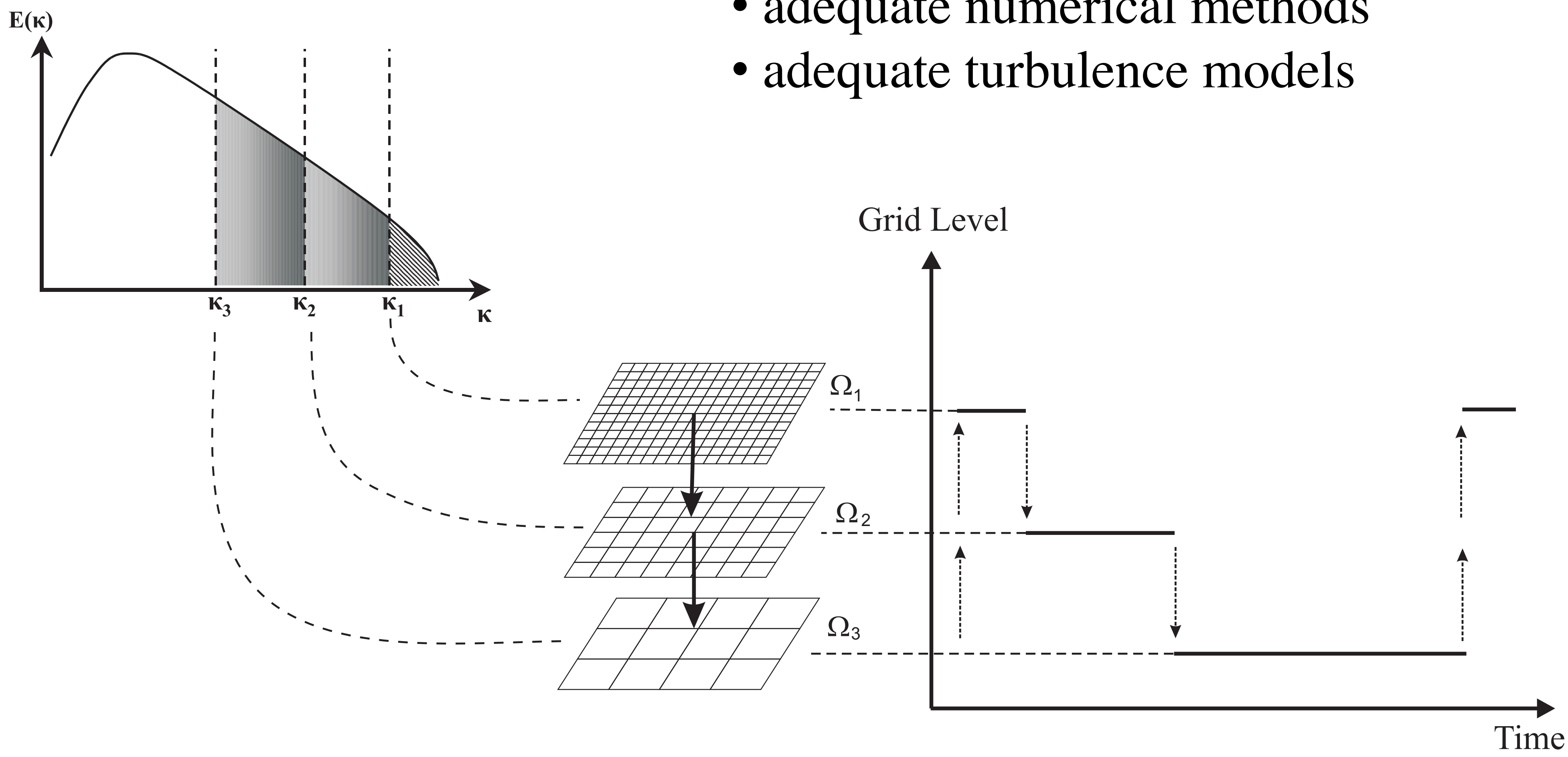
- **Wavelet methods**: CVS *(Schneider, Farge)*, SCALES *(Vasilyev, De Stephano, Goldstein)*

[De Stephano & Vasilyev, JCP 238, 2013]
[De Stephano & Vasilyev, JFM 695, 2012]
[Jarhul et al., Numer. Heat Transfer B 61, 2012]
[De Stephano & Vasilyev, JFM 646, 2010]
[Schneider& Vasilyev, Ann. Rev. Fluid Mech., 2010]
[De Stephano et al., Phys. Fluids 9(11), 2008]
[Goldstein et al., Phys. Fluids 6(71), 2005]
[Goldstein & Vasilyev, Phys. Fluids 16(7), 2004]

Multilevel splitting: schematic view

Related issues:

- time cycling between grids
- reconstruction/restriction operators
- adequate numerical methods
- adequate turbulence models



Vasilyev's Wavelet Method

Wavelet decomposition

Wavelet family loop

Wavelet

$$\mathbf{u}(\mathbf{x}) = \sum_{l \in L_0} c_l^0 \phi_l^0(\mathbf{x}) + \sum_{j=0}^{+\infty} \sum_{m=1}^{2^n-1} \sum_{k \in \mathcal{K}^{m,j}} d_k^{m,j} \psi_k^{m,j}(\mathbf{x})$$

Scaling function

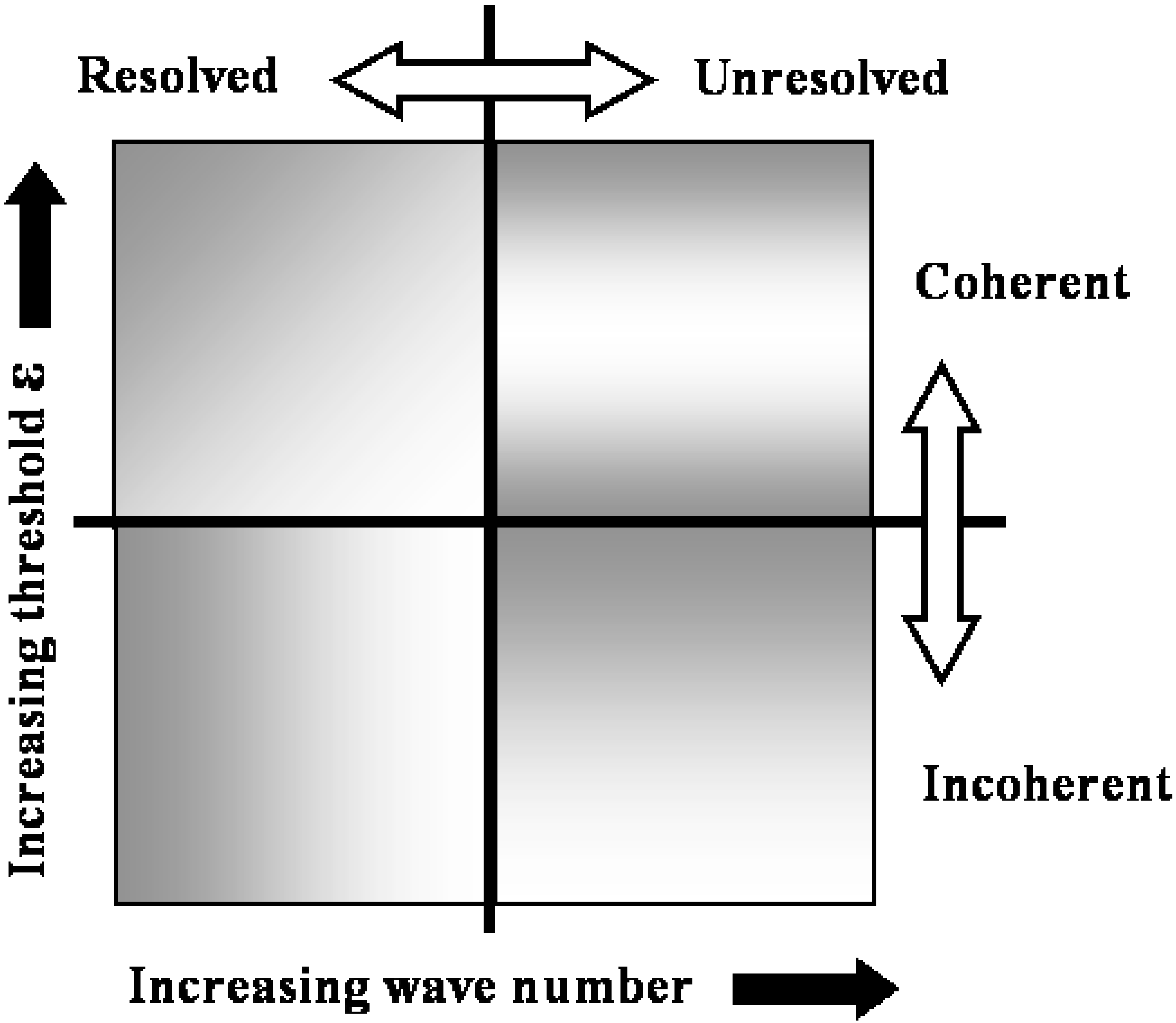
Resolution loop

Degrees of freedom

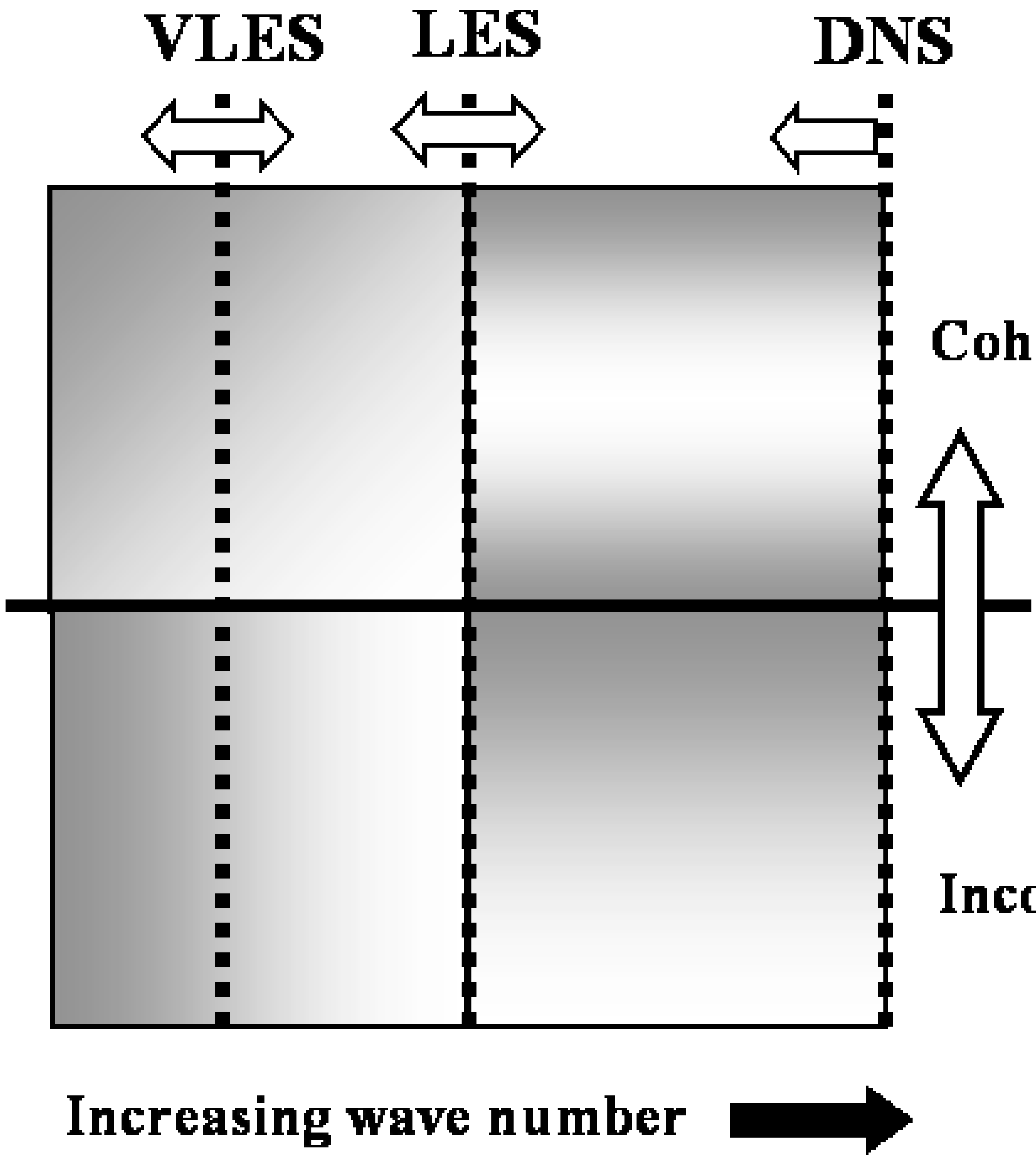
Coherent part

$$\mathbf{u}_>(\mathbf{x}) = \sum_{l \in L_0} c_l^0 \phi_l^0(\mathbf{x}) + \sum_{j=0}^{+\infty} \sum_{m=1}^{2^n-1} \sum_{\substack{k \in \mathcal{K}^{m,j} \\ |d_k^{m,j}| > \epsilon}} d_k^{m,j} \psi_k^{m,j}(\mathbf{x})$$

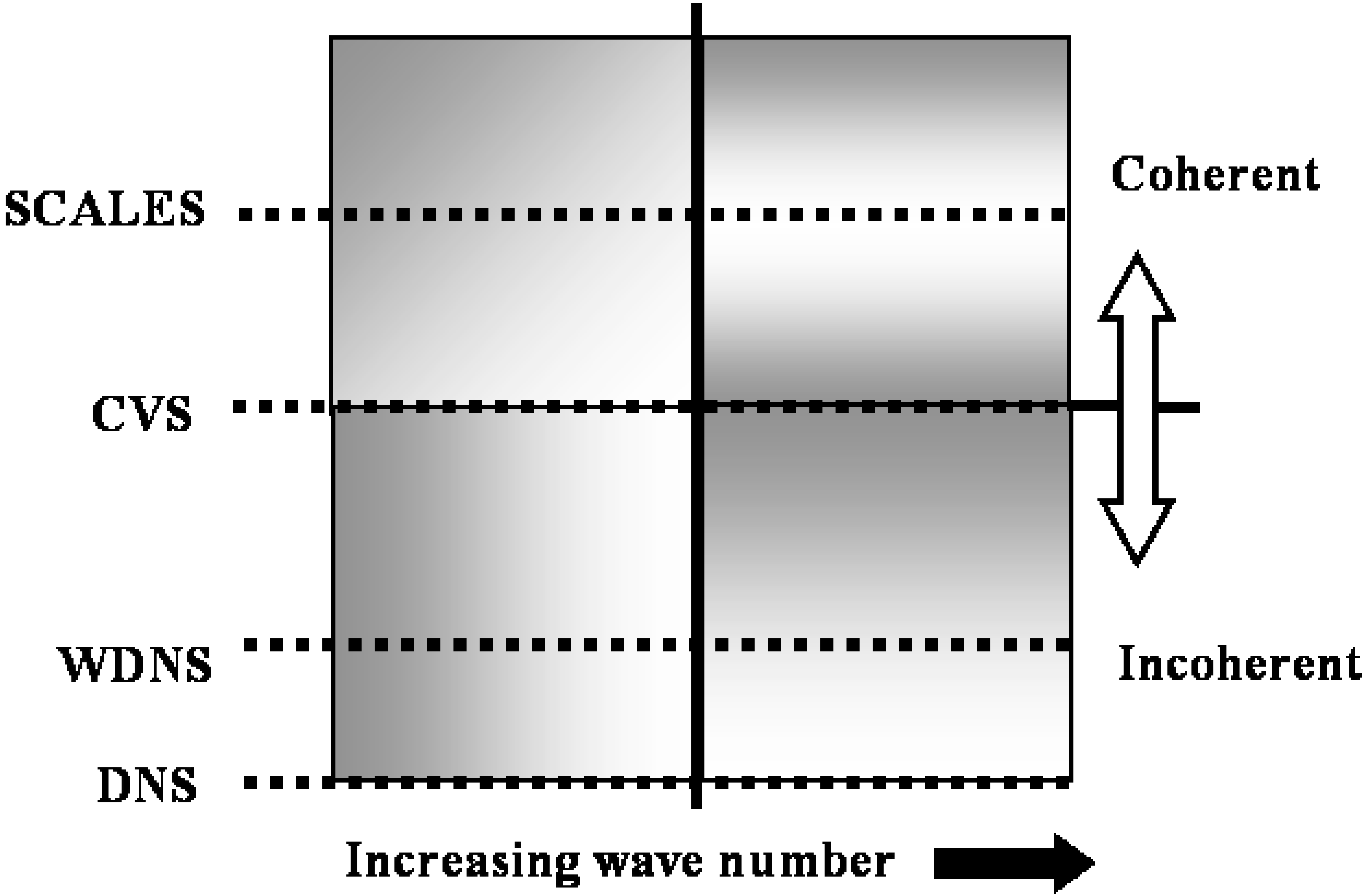
Vasilyev's Wavelet Method



Vasilyev's Wavelet Method



Vasilyev's Wavelet Method



SCALES method governing equations

$$\frac{\partial \overline{\mathbf{u}}^{>\epsilon}}{\partial t} + \nabla \cdot \left(\overline{\mathbf{u}}^{>\epsilon} \otimes \overline{\mathbf{u}}^{>\epsilon}\right) = -\nabla \overline{p}^{>\epsilon} + \nu \nabla^2 \overline{\mathbf{u}}^{>\epsilon} - \nabla \cdot \overline{\tau}^{>\epsilon}$$

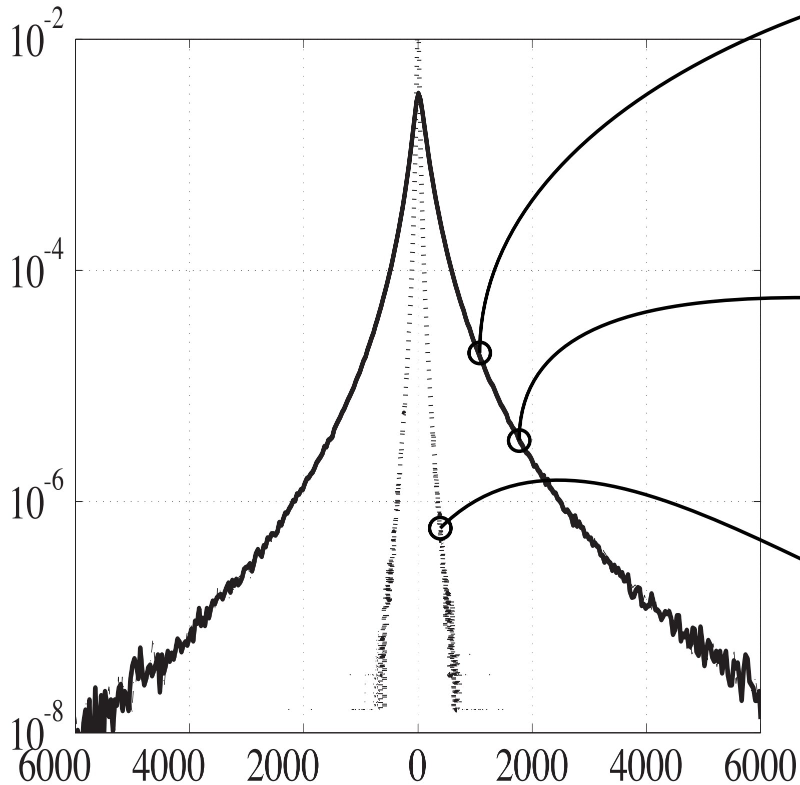
$$\overline{\tau}^{>\epsilon} \equiv \overline{\mathbf{u} \otimes \mathbf{u}}^{>\epsilon} - \overline{\mathbf{u}}^{>\epsilon} \otimes \overline{\mathbf{u}}^{>\epsilon}$$

$$\overline{\tau}^{>\epsilon} = -2\nu_{\text{scales}} \overline{\mathbf{S}}^{>\epsilon}, \quad \overline{S}^{>\epsilon} = \frac{1}{2}\left(\nabla \overline{\mathbf{u}}^{>\epsilon} + \nabla^T \overline{\mathbf{u}}^{>\epsilon}\right)$$

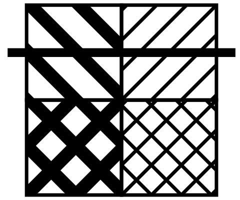
$$\nu_{\text{scales}} = C_S \epsilon^2 |\overline{\mathbf{S}}^{>\epsilon}|.$$

Dissipation in isotropic turbulence

$$PDF : -\tau_{ij}\overline{S}_{ij}$$



SCALES (*21267 resolved modes*)

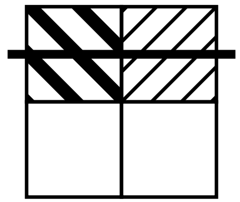


$Mean/\varepsilon = 0.552$

$\sigma/\varepsilon = 4.700$

$Mean/\sigma = 0.118$

SCALES, Coherent SGS (*5%*)

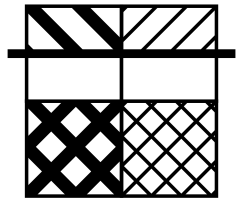


$Mean/\varepsilon = 0.549$

$\sigma/\varepsilon = 4.709$

$Mean/\sigma = 0.117$

SCALES, Incoherent SGS (*95%*)

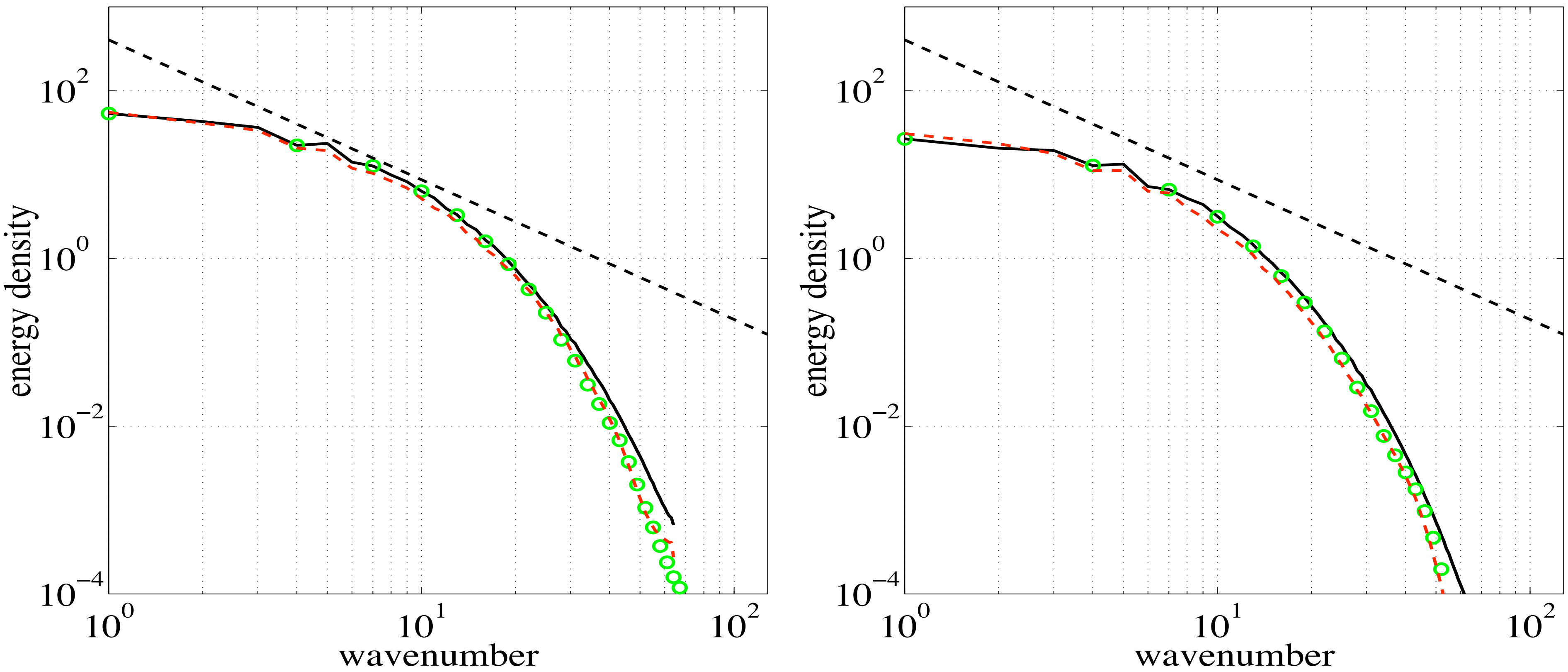


$Mean/\varepsilon = 0.00321$

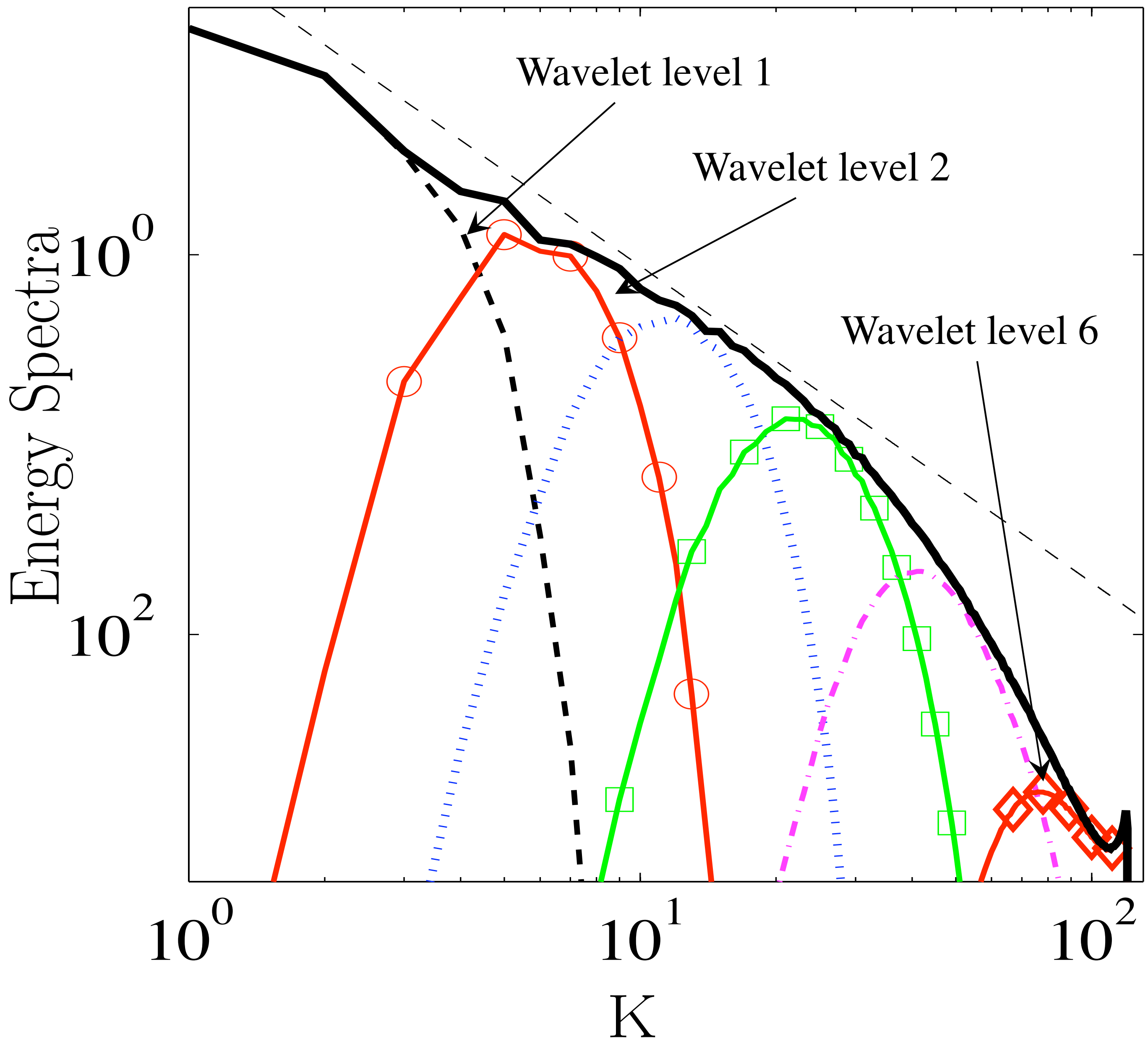
$\sigma/\varepsilon = 0.390$

$Mean/\sigma = 0.00823$

Computed energy spectrum



Computed energy spectrum



Hoffman's AMR DNS/LES

Key idea: error dynamics interpreted using (non)linear stability theory

[Huerre & Monkewitz, Ann. Rev. Fluid Mech, 1990]

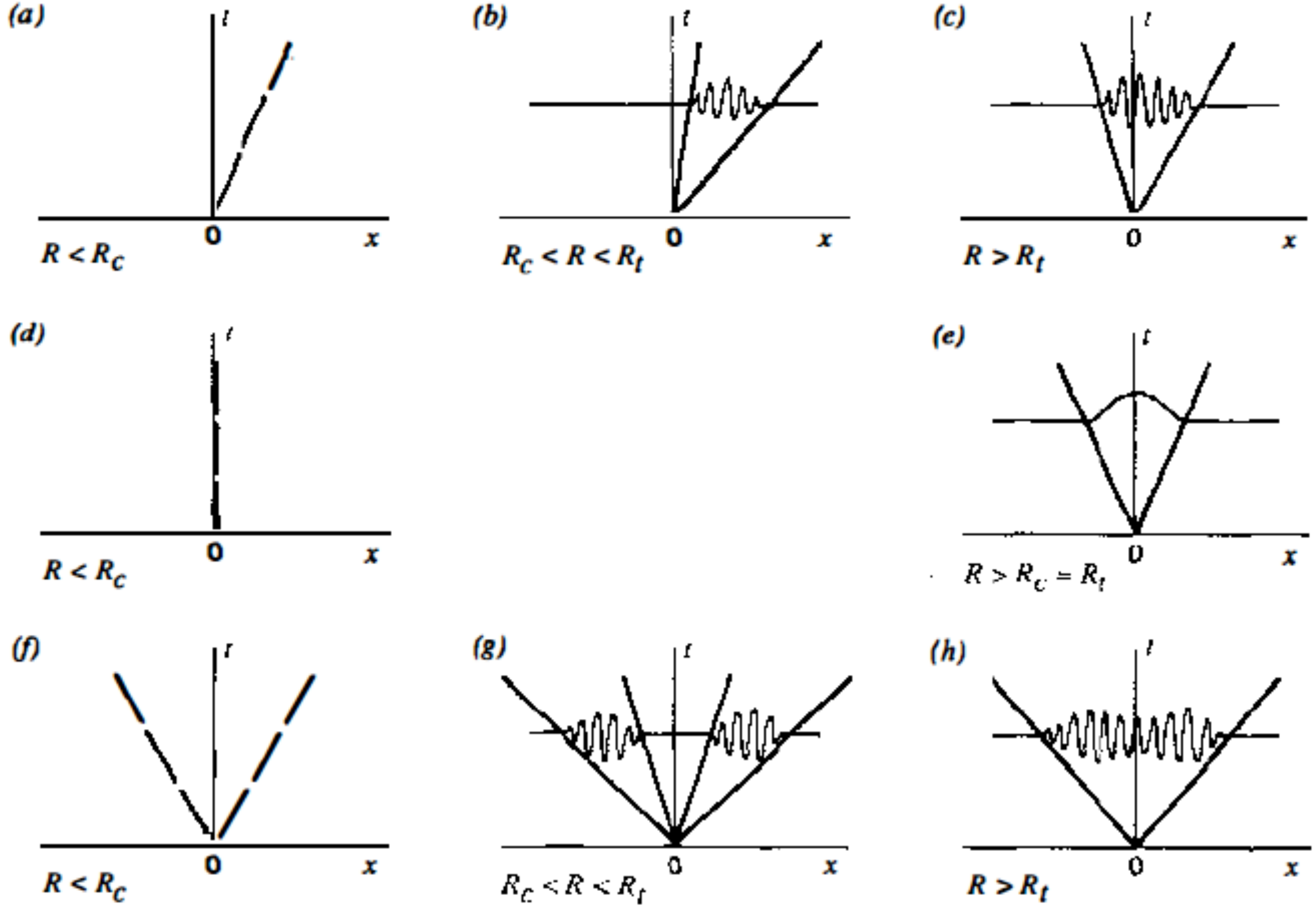
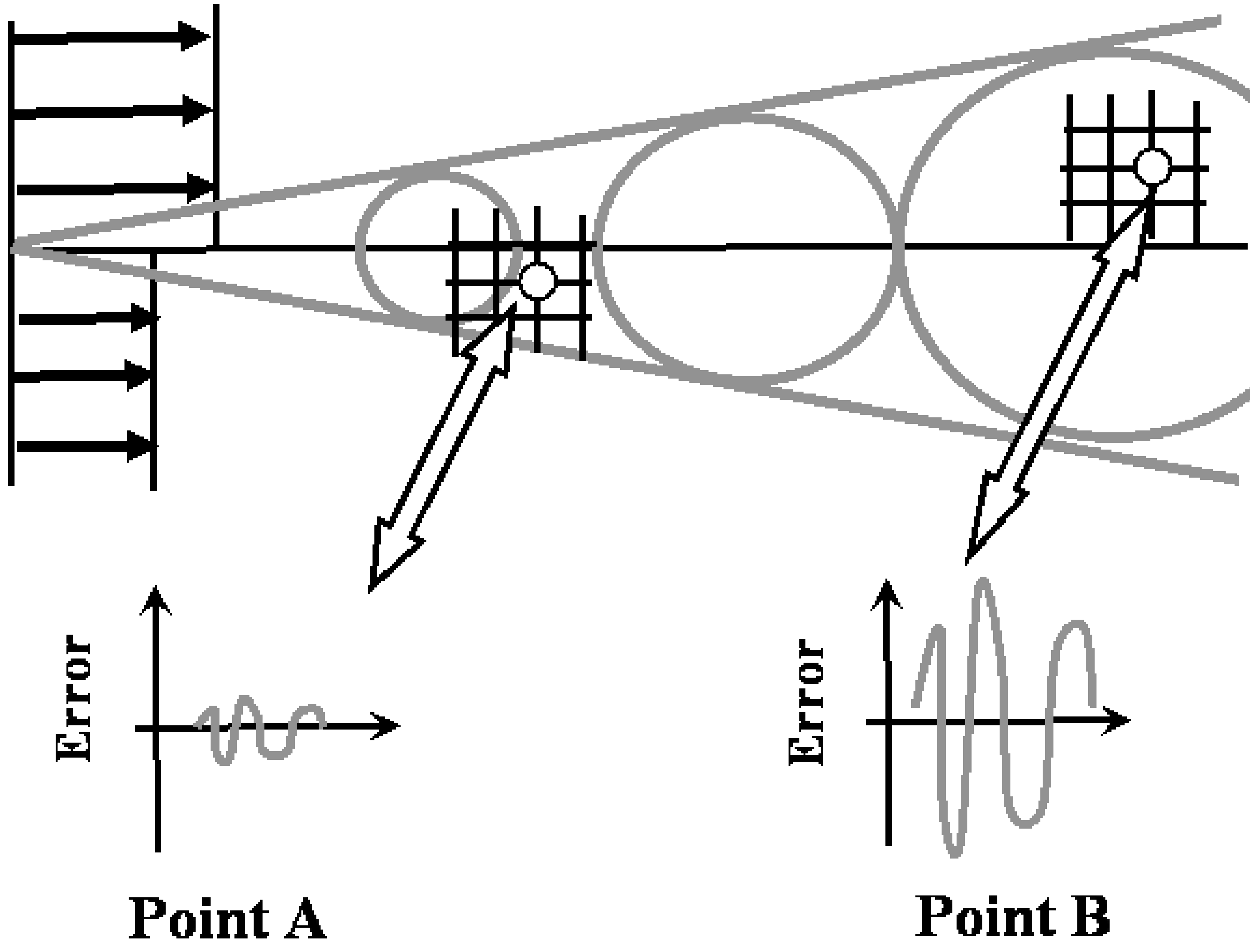


Figure 1 Sketches of typical impulse responses. Single traveling wave: (*a*) stable, (*b*) convectively unstable, (*c*) absolutely unstable. Stationary mode: (*d*) stable, (*e*) absolutely unstable. Counterpropagating traveling waves: (*f*) stable, (*g*) convectively unstable, (*h*) absolutely unstable.

Hoffman's AMR DNS/LES

Key idea: convective nature of error in noise amplificator flows



Hoffman's AMR DNS/LES

Hoffman's error cost function

Time-averaged Drag function (local/surfacic formulation)

$$F(\sigma(\mathbf{u},p)) \equiv \frac{1}{T}\int_I \int_{\Gamma_0} (\sigma \cdot \mathbf{n}) \cdot \phi \, dS \, dt$$

Time-averaged Drag function (non-local/volumic formulation)

$$F(\sigma(\mathbf{u},p)) \equiv \frac{1}{T}\int_I \left(\langle \dot{\mathbf{u}} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}), \mathbf{\Phi} \rangle + \langle p, \nabla \cdot \mathbf{\Phi} \rangle \right.$$
$$\left. + 2\nu \, \langle S(\mathbf{u}), S(\mathbf{\Phi}) \rangle + \langle \nabla \cdot \mathbf{u}, \Theta \rangle \right) dt$$

Hoffman's AMR DNS/LES

Hoffman's error cost function

Time-averaged Drag function (volumic discrete formulation)

$$
\begin{aligned}
F_h(\sigma(\mathbf{u}_h, p_h)) \equiv \quad & \frac{1}{T}\int_I \left(\langle \dot{\mathbf{u}}_h + \nabla\cdot(\mathbf{u}_h \otimes \mathbf{u}_h), \mathbf{\Phi}\rangle + \langle p_h, \nabla\cdot\mathbf{\Phi}\rangle \right. \\
& + 2\nu \langle S(\mathbf{u}_h), S(\mathbf{\Phi})\rangle + \langle \nabla\cdot\mathbf{u}_h, \Theta\rangle \\
& \left. + \mathrm{SGS}(h, \mathbf{u}_h, p_h, \mathbf{\Phi}, \Theta) \right) dt
\end{aligned}
$$

Drag error cost function

$$
\mathrm{Err}(h_r, \lambda) = |F(\sigma(\mathbf{u}, p)) - F_h(\sigma(\mathbf{u}_h, p_h))|
$$

Hoffman's AMR DNS/LES

Optimal AMR: adjoint-based grid refinement

$$-\frac{\partial \phi}{\partial t} - \mathbf{u} \cdot \nabla \phi = \nabla \theta + \nu \nabla^2 \phi - \nabla \mathbf{u}_h \cdot \phi$$

$$\nabla \cdot \phi = 0$$

Drag error cost function

$$|F(\sigma(\mathbf{u}, p)) - F_h(\sigma(\mathbf{u}_h, p_h))| = \left| \sum_{i=1,N} \mathrm{Err}_h(i) + \sum_{i=1,N} \mathrm{Err}_r(i) \right|$$

Hoffman's AMR DNS/LES

Drag error cost function: local discretization error

$$\mathrm{Err}_h(i) = \frac{1}{T}\int_I \Big(\langle \dot{\mathbf{u}}_h + \nabla\cdot(\mathbf{u}_h \otimes \mathbf{u}_h), (\phi_h - \mathbf{\Phi})\rangle_i + \langle p_h, \nabla\cdot(\phi_h - \mathbf{\Phi})\rangle_i + 2\nu\, \langle S(\mathbf{u}_h), S(\phi_h - \mathbf{\Phi})\rangle + \langle \nabla\cdot\mathbf{u}_h, (\theta_h - \Theta)\rangle_i \Big)\, dt$$

Drag error cost function: resolution/modelling error

$$\mathrm{Err}_r(i) = \frac{1}{T}\int_I \mathrm{SGS}(h, \mathbf{u}_h, p_h, \mathbf{\Phi}, \Theta)_i dt$$

Several solutions for resolution error definition

Hoffman's AMR DNS/LES

Drag error cost function: resolution/modelling error

$$\mathrm{Err}_r(i) = \frac{1}{T}\int_I \mathrm{SGS}(h, \mathbf{u}_h, p_h, \mathbf{\Phi}, \Theta)_i dt$$

DNS as a target

$$\mathrm{SGS}(h, \mathbf{u}_h, p_h, \mathbf{\Phi}, \Theta)_i = \langle \mathcal{F}_{\mathrm{LES}}, \mathbf{\Phi} \rangle_i$$

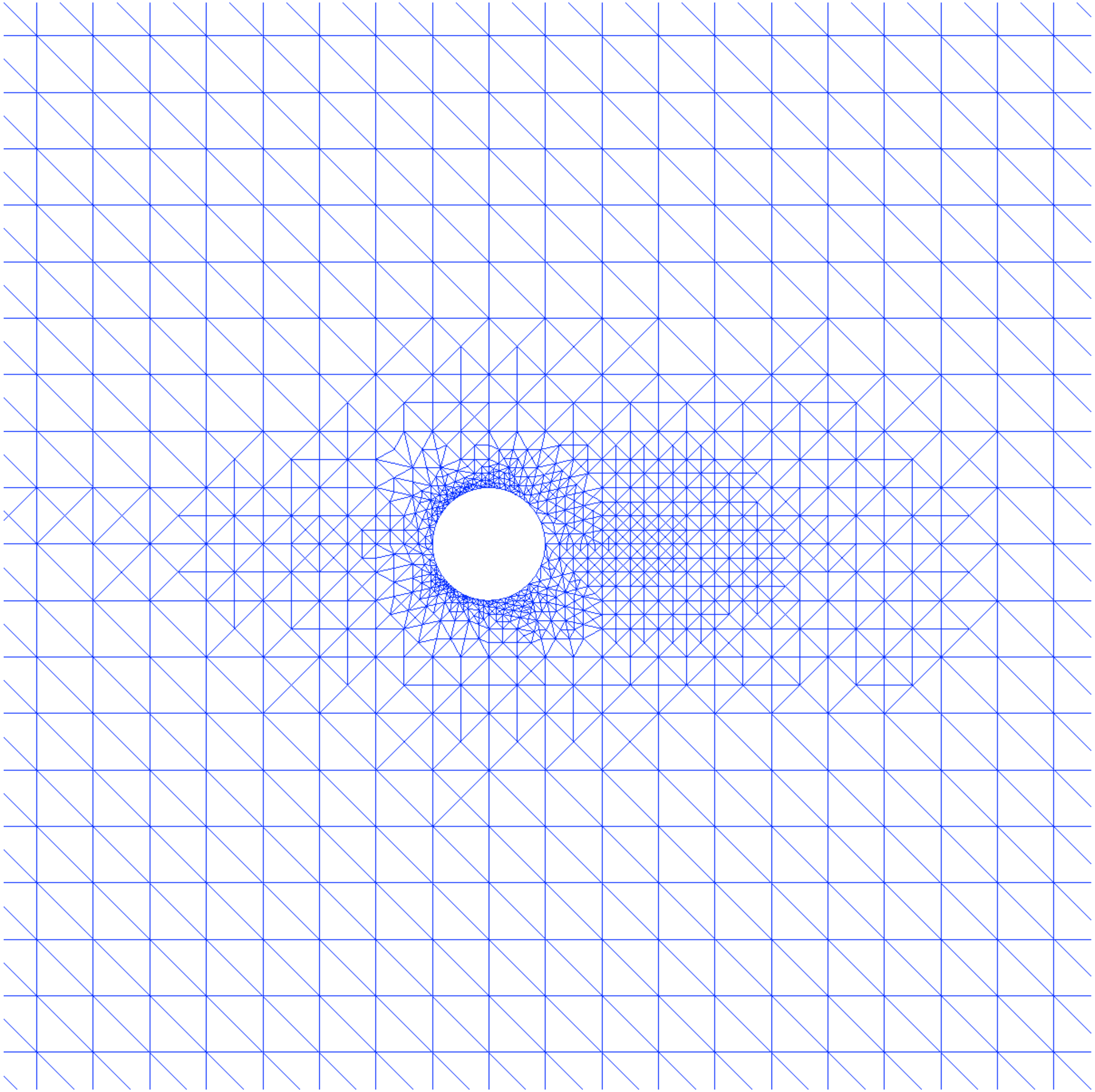
$$(\mathbf{\Phi}, \Theta) = (\phi_h, \theta_h)$$ Test on sugrid force (weak form)

$$(\mathbf{\Phi}, \Theta) = (\mathbf{u}_h, p_h)$$ Test on sugrid dissipation

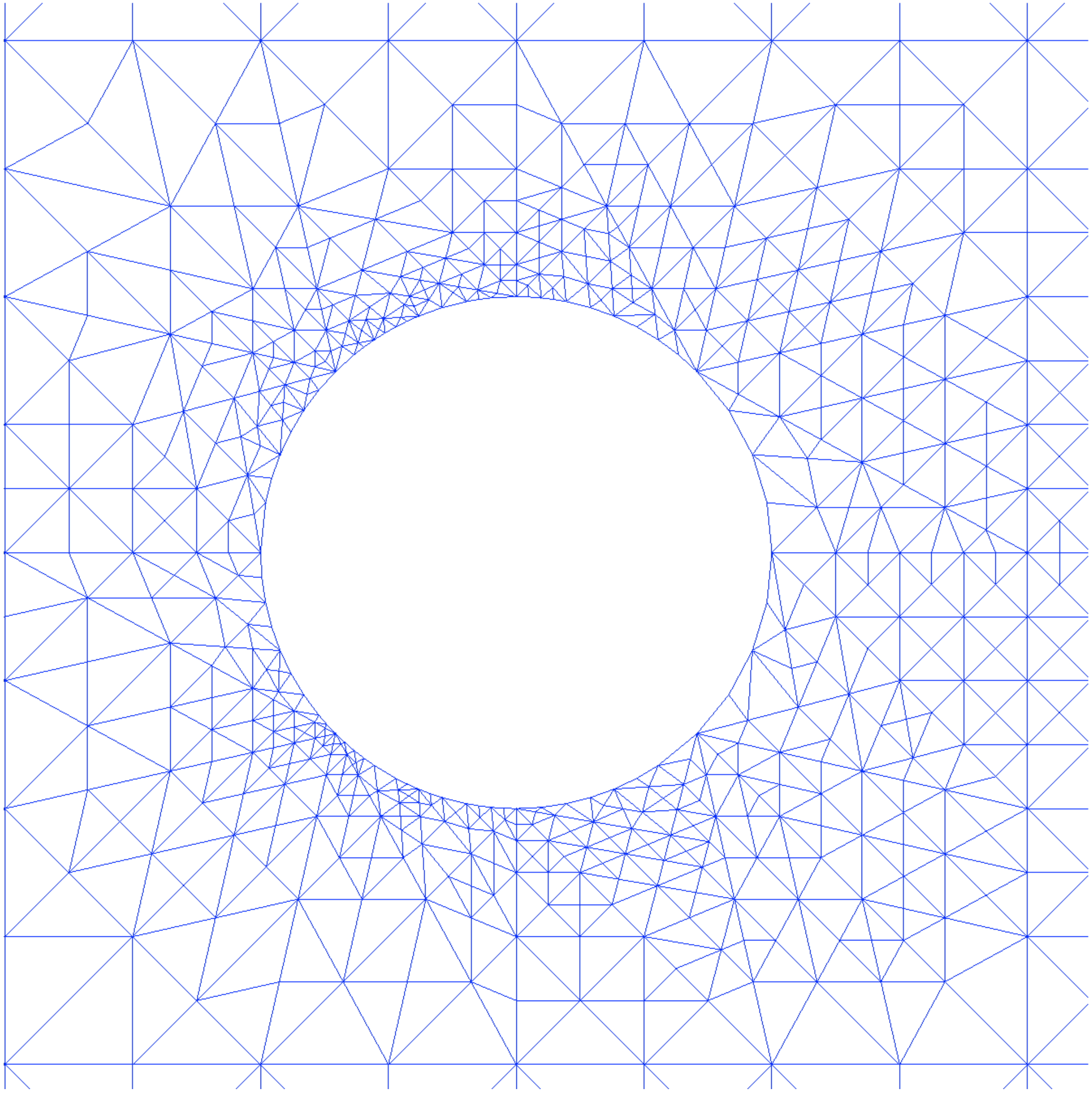
Ideal filtered DNS as a target

$$\begin{aligned}\mathrm{SGS}(h, \mathbf{u}_h, p_h, \mathbf{\Phi}, \Theta)_i &= \langle \nabla \cdot \tau_{\mathrm{LES}} - \mathcal{F}_{\mathrm{LES}}, \mathbf{\Phi} \rangle_i \\ &= \langle \tau_{\mathrm{LES}}, S(\mathbf{\Phi}) \rangle_i - \langle \mathcal{F}_{\mathrm{LES}}, \mathbf{\Phi} \rangle_i\end{aligned}$$

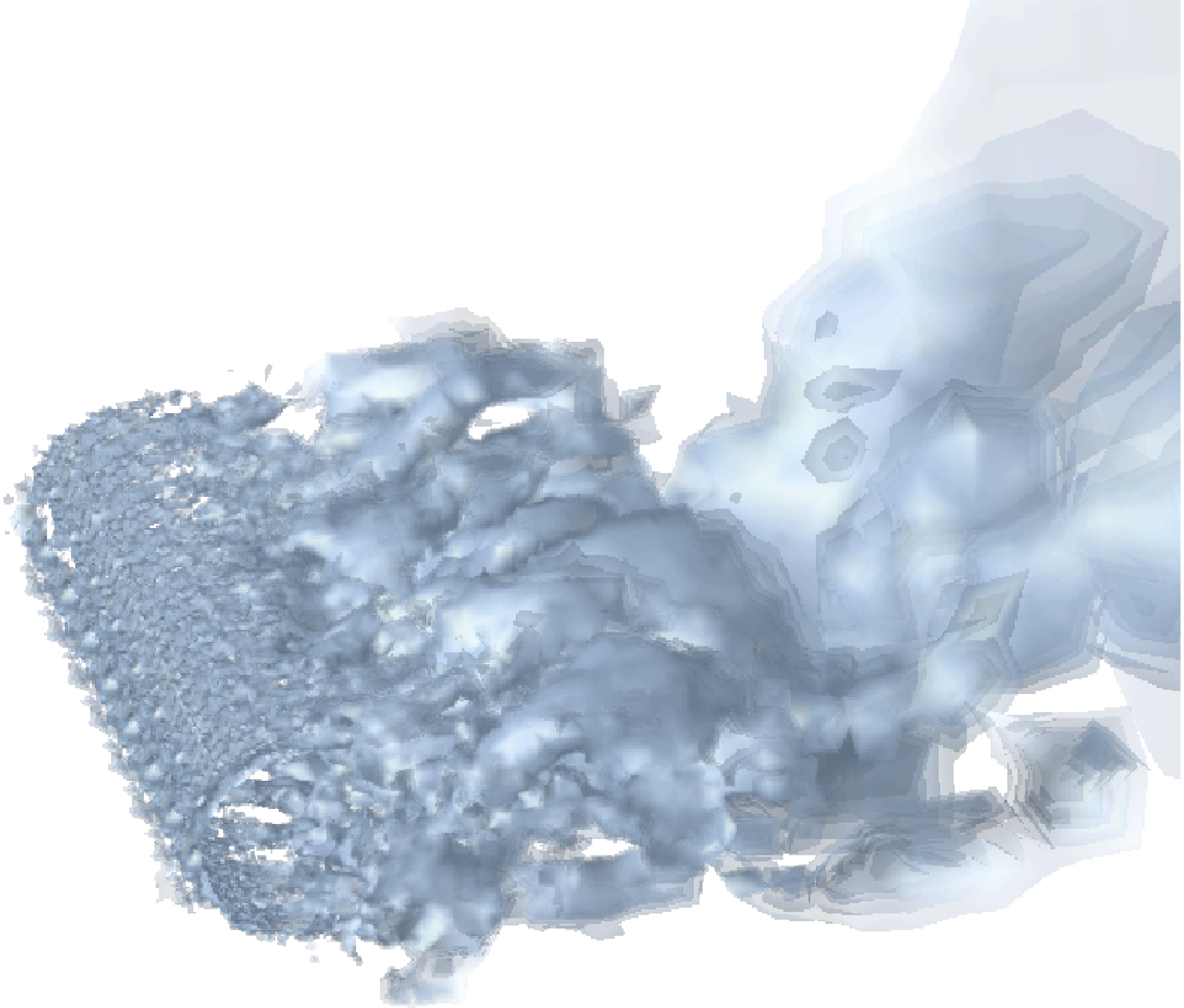
Hoffmann’s AMR DNS/LES



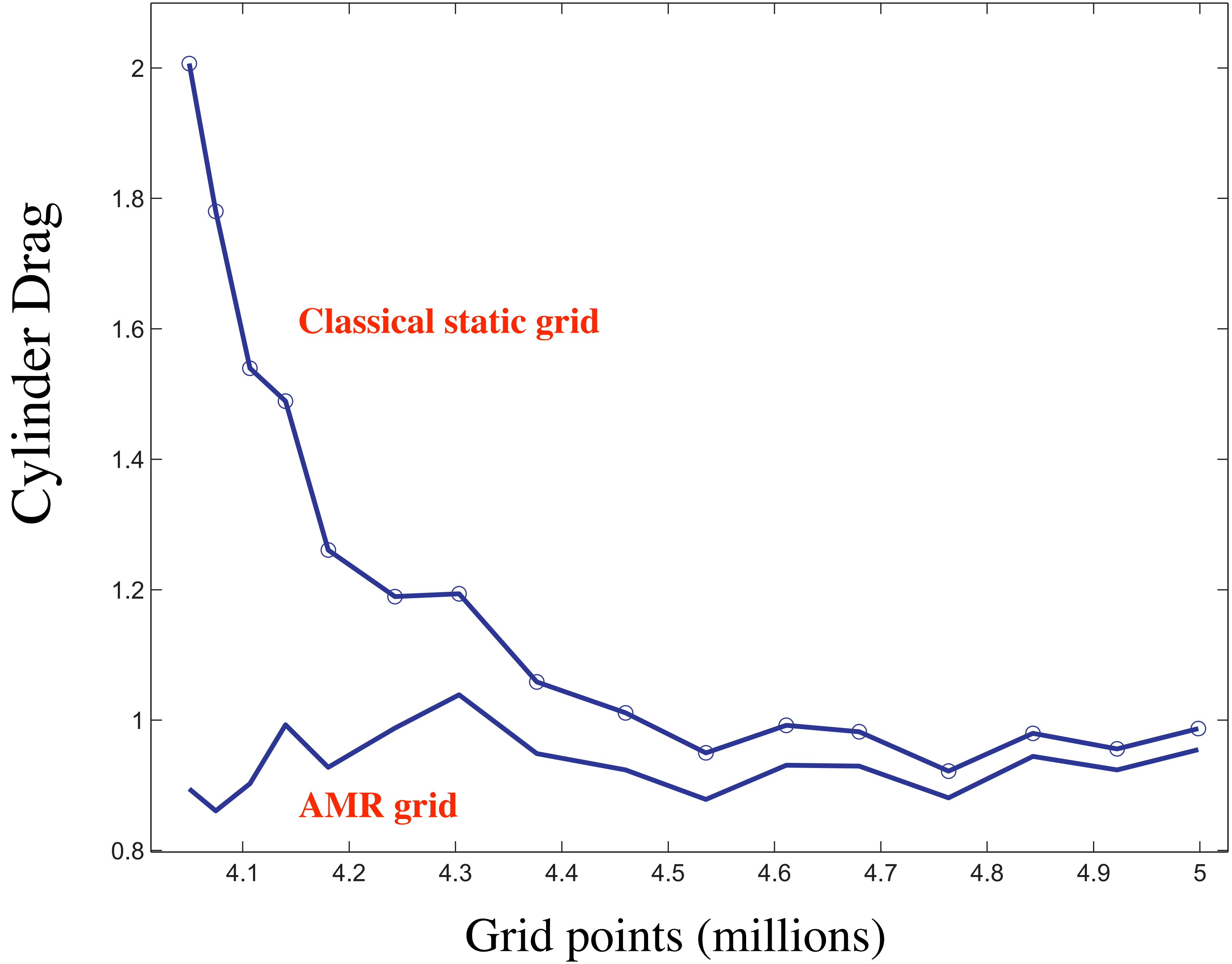
Hoffmann's AMR DNS/LES



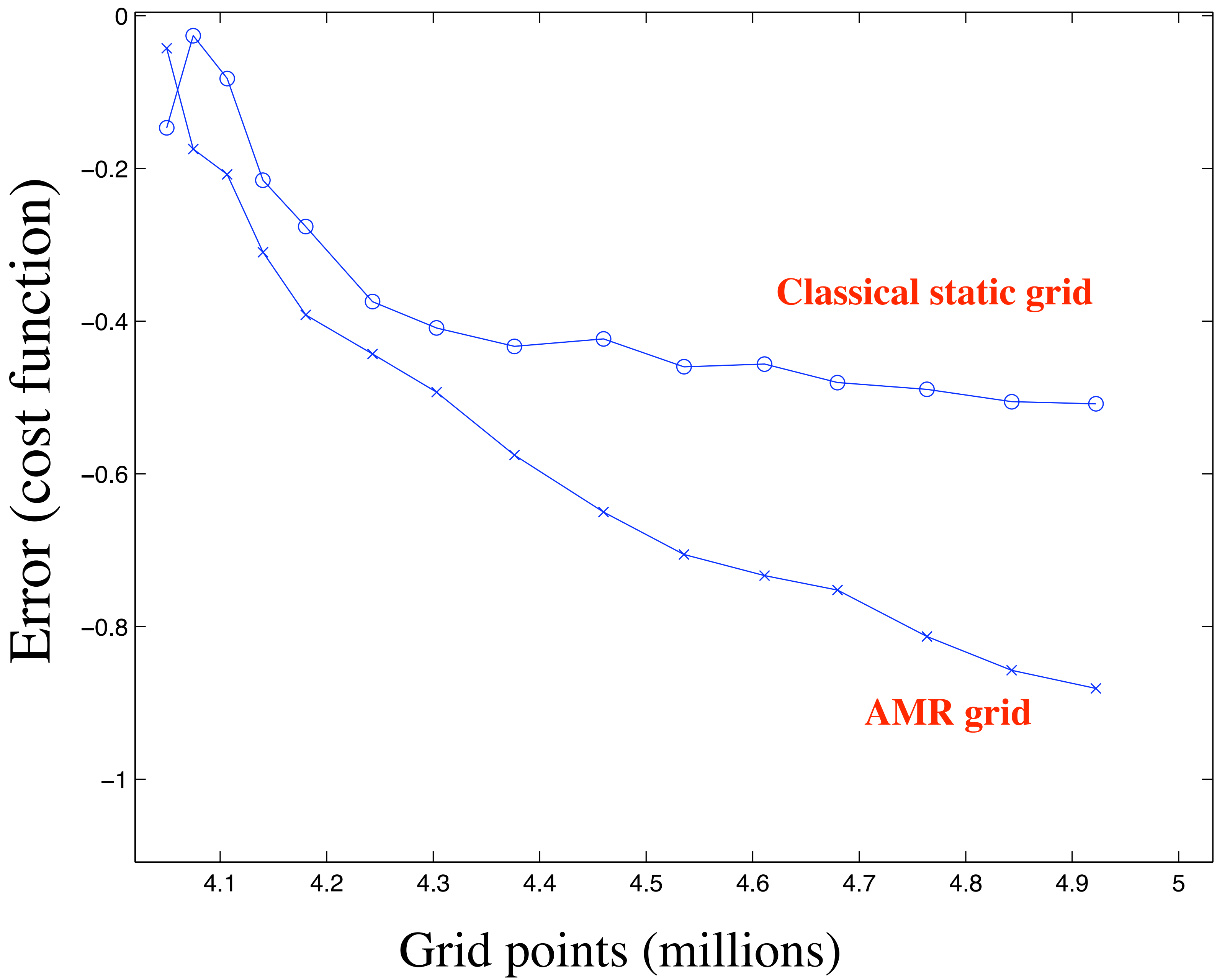
Hoffmann's AMR DNS/LES



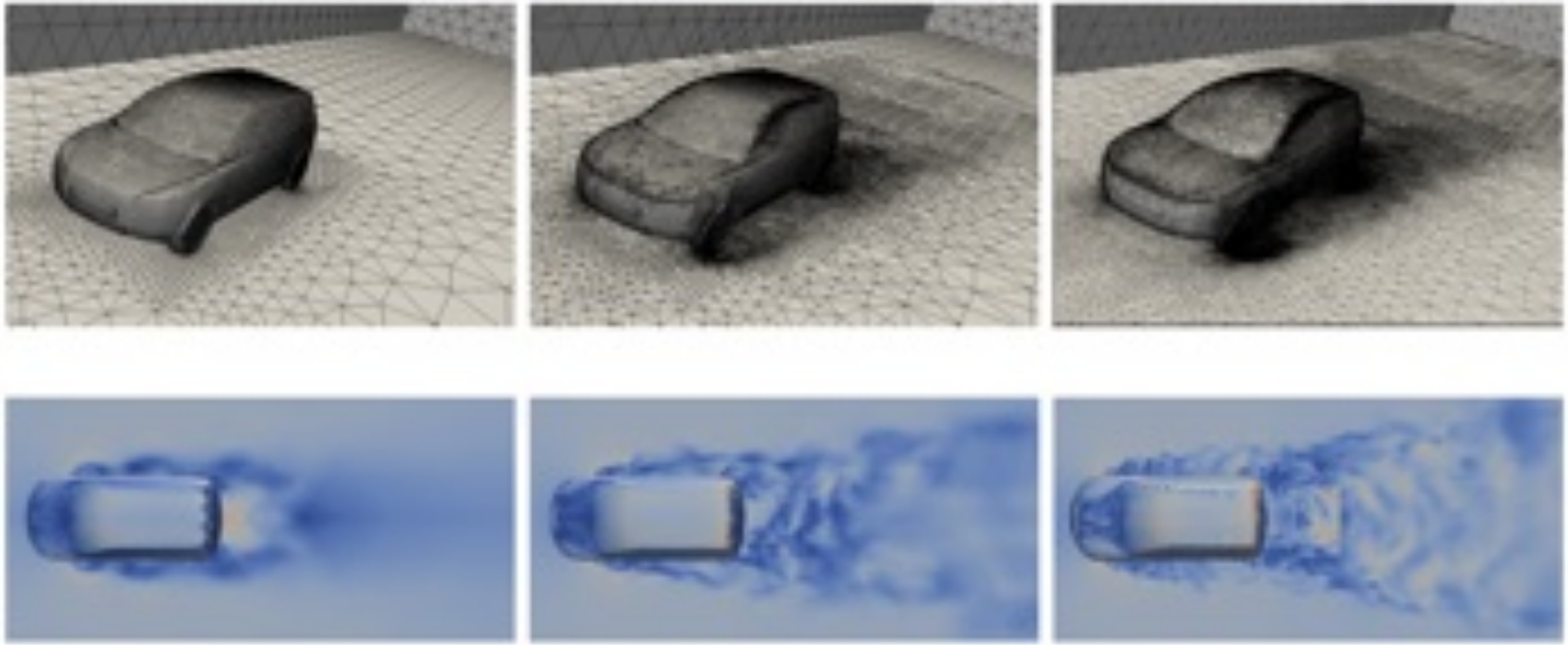
Hoffmann's AMR DNS/LES



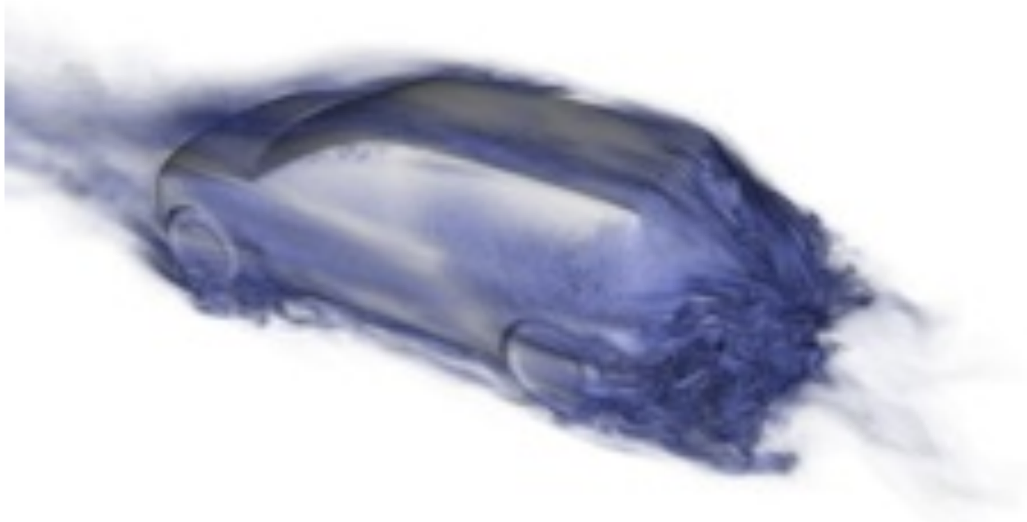
Hoffmann's AMR DNS/LES



Engineering applications

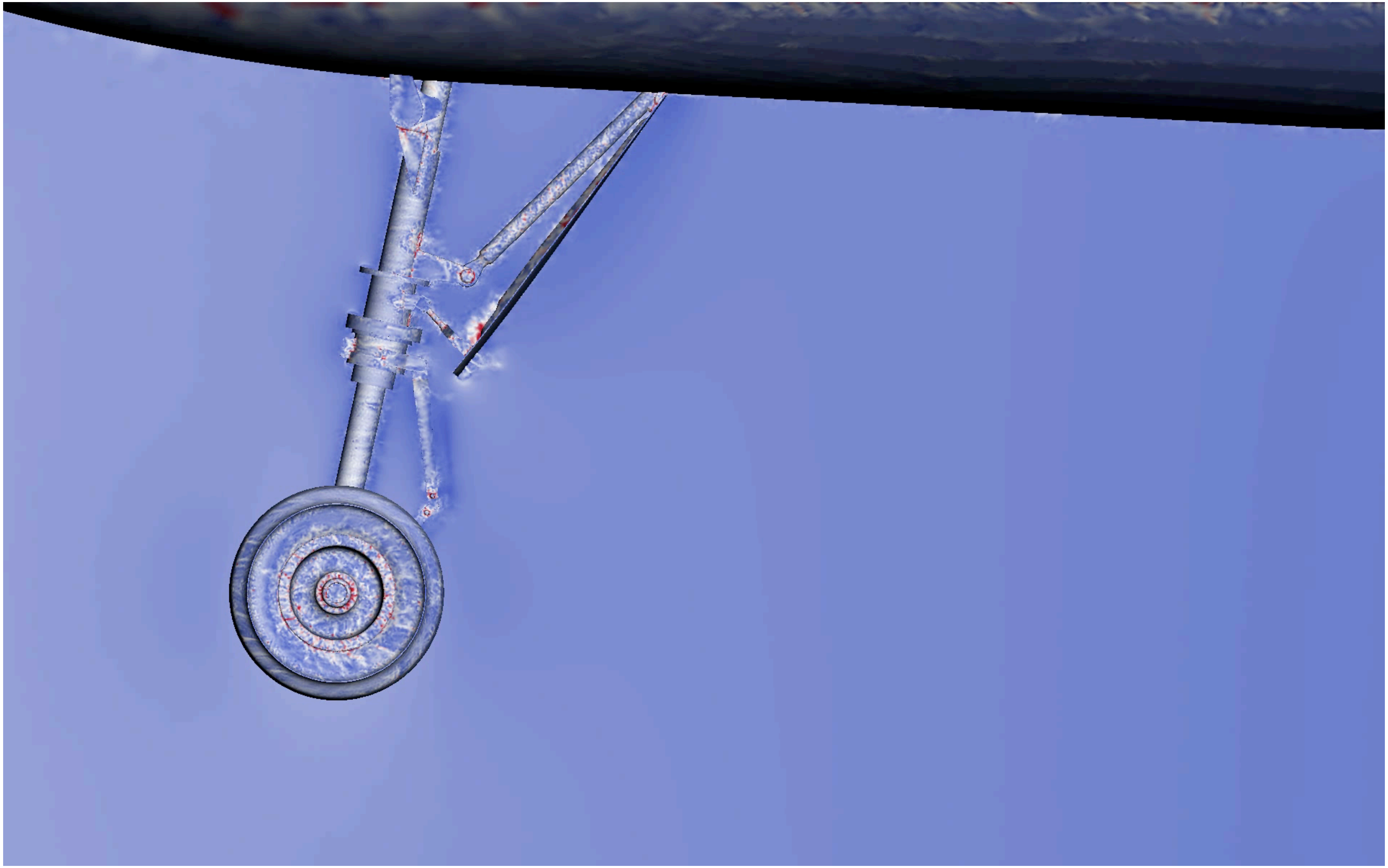


Adjoint solution



Engineering applications

Engineering applications



AMR vs. LES (modelling)

	pros	cons
AMR	• no physical modelling • fully general • reduced numerical error	• error estimate needed • no fully general error estimate • non-conformal grids • conservation properties • dynamic load distribution on // computers • arbitrary maximum resolution (high-Re DNS ?)
LES (modelling)	• static grid (general case) • huge effort over 40 years • some reliable/robust methods are available	• empirical physical modelling • models limited to cascade +dissipation: no production • models restricted to almost isotropic subgrid physics • empirical handling of numerical errors

AMR vs. LES (modelling)

- Hybrid LES/AMR methods seem to be preferred in engineering
- Optimal weight grid/model complexity still unknown
- How to distinguish between numerical and modelling errors ?
- How to capture governing/production mechanisms at very small scales (e.g. chemical reaction at molecular scales) ?

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