

Going beyond eddy viscosity:
Finding a general representation of subgrid-scale stresses
in large-eddy simulation



Maurits Silvis

Supervisors

Roel Verstappen

Arthur Veldman

JMBC Turbulence Contact
group

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university of
 groningen

faculty of mathematics
and natural sciences

johann bernoulli institute for
mathematics and computer science

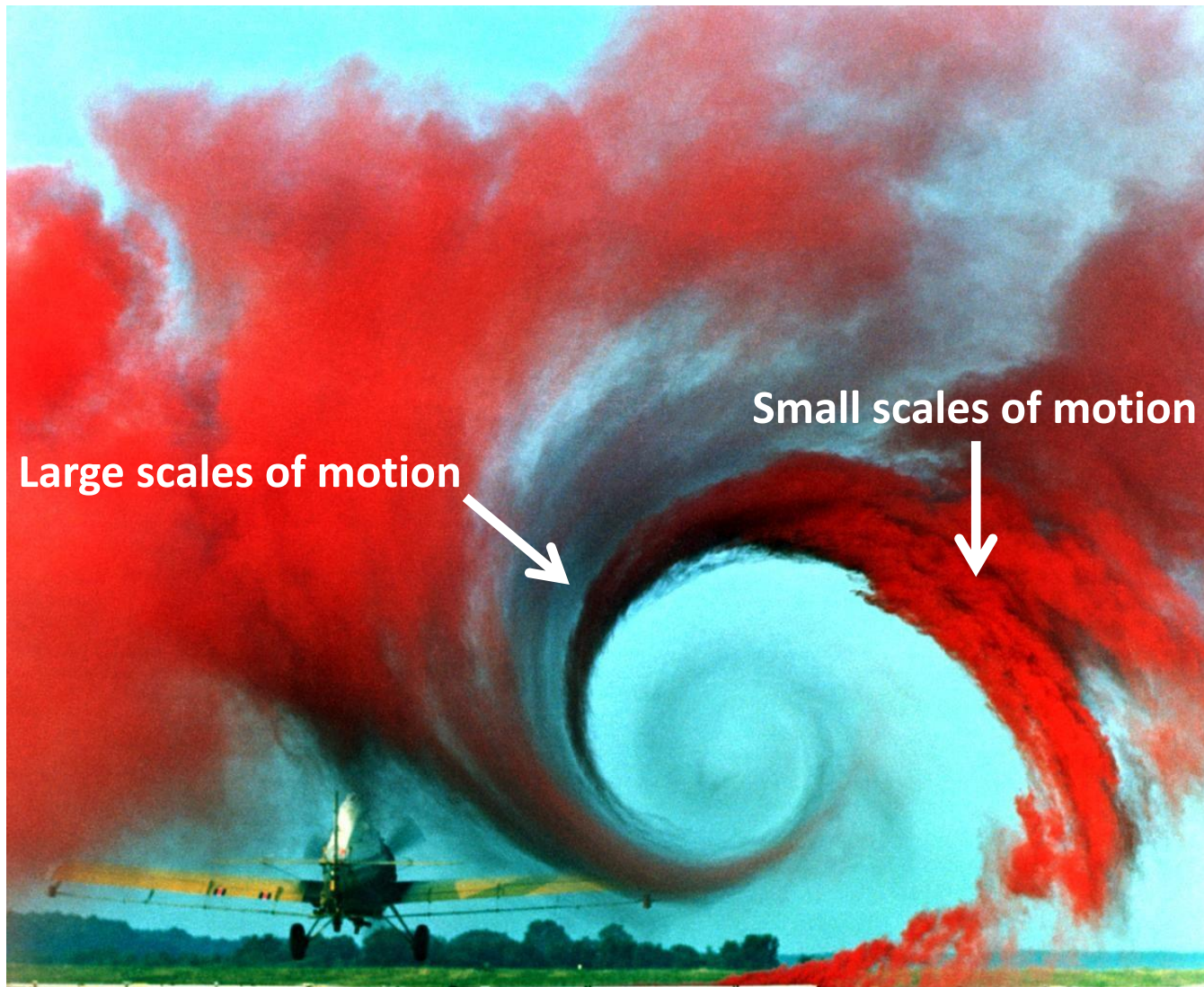
Overview

- Goal: describe and predict the behavior of turbulent flows
- Tool: large-eddy simulation

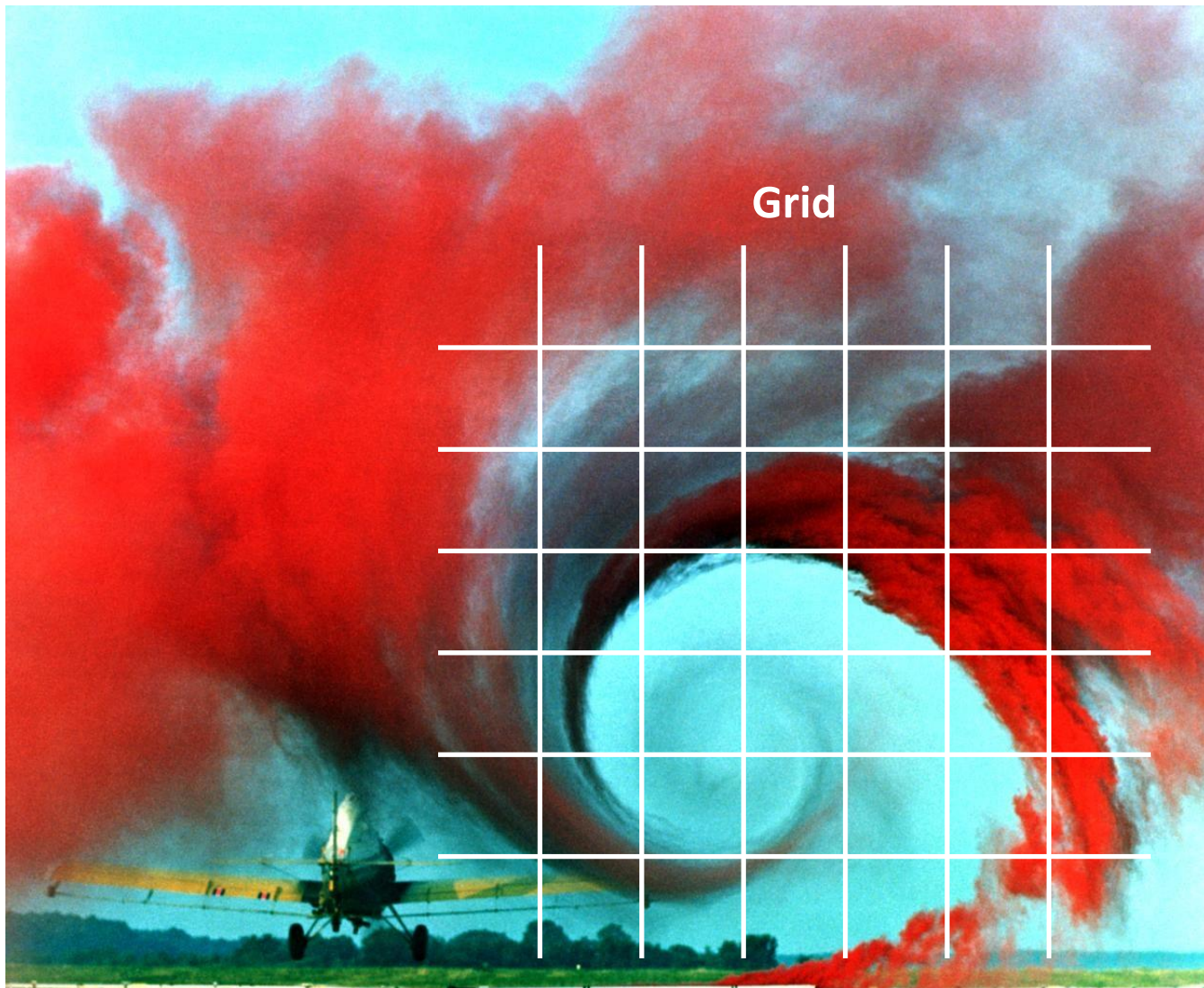
- Goal: improve on the purely dissipative description
- Tool: nonlinear model

- Today's topics:
 - Construction of a general nonlinear model for large-eddy simulation
 - Discussion of physical constraints, applied to the model

Describing turbulent flows



Describing turbulent flows



Large-eddy simulation

- Filtered Navier-Stokes equations

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j} \tau_{ij}$$

- Describe evolution of large-scale motions

- Closure problem

- $\tau_{ij} = \overline{u_i u_j} - \bar{u}_i \bar{u}_j$ unknown
- Provide closure / subgrid-scale model:

$$\tau \approx \tau^{mod}$$

Here: in terms of \bar{u}_i and derivatives

Examples of subgrid-scale models

- Building blocks $\bar{S}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)$, $\bar{\Omega}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} - \frac{\partial \bar{u}_j}{\partial x_i} \right)$

- Eddy viscosity models

$$\tau^{mod} - \frac{1}{3} \text{tr}(\tau^{mod}) I = -2\nu_e \bar{S}$$

- + Mean dissipation of energy can be captured
- Backscatter not captured very well, structure of τ modeled incorrectly

- The gradient / nonlinear model

$$\tau^{mod} = C \nabla \bar{u} (\nabla \bar{u})^T = C (\bar{S}^2 - \bar{\Omega}^2 - (\bar{S} \bar{\Omega} - \bar{\Omega} \bar{S}))$$

- + Structure of τ captured better
- Not dissipative enough, unstable

- More general nonlinear models

Winckelmans et al. (2001), *Phys. Fluids* **13**, 5

Vreman, Geurts and Kuerten (1996), *Theor. Comp. Fluid Dyn.* **8**, 309

Tao et al. (2002), *J. Fluid Mech.* **457**, 35

Horiuti (2001), *Direct and Large Eddy-Simulation IV*, 67

Assumptions

- Filtered velocity gradient determines subgrid stresses

$$\tau^{mod} = f(\bar{S}, \bar{\Omega})$$

- Condition of isotropy

$$Q\tau^{mod}Q^T = f(Q\bar{S}Q^T, Q\bar{\Omega}Q^T)$$

- Orthogonal transformation of coordinate system: Q

- Resulting model: general polynomial

- Terms: $\bar{S}^{m_1}\bar{\Omega}^{n_1}\bar{S}^{m_2}\bar{\Omega}^{n_2} \dots$

- Coefficients: depending on scalar invariants of terms

Cayley-Hamilton theorem

- Resulting model: $\tau^{mod} = \sum_{i=0}^{10} \alpha_i T_i$

– Terms T_i :

$$T_0 = I$$

$$T_1 = \bar{S}$$

$$T_2 = \bar{S}^2$$

$$T_3 = \bar{\Omega}^2$$

$$T_4 = \bar{S} \bar{\Omega} - \bar{\Omega} \bar{S}$$

$$T_5 = \bar{S}^2 \bar{\Omega} - \bar{\Omega} \bar{S}^2$$

$$T_6 = \bar{S} \bar{\Omega}^2 + \bar{\Omega}^2 \bar{S}$$

$$T_7 = \bar{\Omega} \bar{S} \bar{\Omega}^2 - \bar{\Omega}^2 \bar{S} \bar{\Omega}$$

$$T_8 = \bar{S} \bar{\Omega} \bar{S}^2 - \bar{S}^2 \bar{\Omega} \bar{S}$$

$$T_9 = \bar{S}^2 \bar{\Omega}^2 + \bar{\Omega}^2 \bar{S}^2$$

$$T_{10} = \bar{\Omega} \bar{S}^2 \bar{\Omega}^2 - \bar{\Omega}^2 \bar{S}^2 \bar{\Omega}$$

– Coefficients α_i depending on scalar invariants:

$$I_1 = \text{tr}(\bar{S}^2)$$

$$I_2 = \text{tr}(\bar{\Omega}^2)$$

$$I_3 = \text{tr}(\bar{S}^3)$$

$$I_4 = \text{tr}(\bar{S} \bar{\Omega}^2)$$

$$I_5 = \text{tr}(\bar{S}^2 \bar{\Omega}^2)$$

$$I_6 = \text{tr}(\bar{S}^2 \bar{\Omega}^2 \bar{S} \bar{\Omega})$$

- Complexity of model

– Practical simulations

– Number of terms

Gram-Schmidt orthogonalization

- Process

$$\begin{array}{l}
 T_0 = I \\
 T_1 = \bar{S} \\
 T_2 = \bar{S}^2 \\
 T_3 = \bar{\Omega}^2 \\
 \vdots
 \end{array}
 \longrightarrow
 \begin{array}{l}
 T'_0 = I \\
 T'_1 = \bar{S} \\
 T'_2 = \bar{S}^2 - \frac{1}{3}I_1T'_0 - \frac{I_3}{I_1}T'_1 \\
 T'_3 = \bar{\Omega}^2 - \frac{1}{3}I_2T'_0 - \frac{I_4}{I_2}T'_1 - \dots T'_2 \\
 \vdots
 \end{array}
 \left. \vphantom{\begin{array}{l} T'_2 \\ T'_3 \\ \vdots \end{array}} \right\} \text{Beyond eddy viscosity}$$

- Results

- T'_8, T'_9, T'_{10} always zero
 - At least two other tensors also zero
 - Independence of terms, mathematically and physically
- } Usually a general representation of τ^{mod}

Results

- General nonlinear model: $\tau^{mod} = \sum_{i=0}^7 \alpha_i' T_i'$
 - At least two tensors zero: usually a general representation of τ^{mod}
 - Independence of terms, mathematically and physically
- Goal:
 - Understand the functional dependence of the coefficients on flow properties
 - Understand the behavior of the different terms

Symmetry requirements

- Symmetries of the Navier-Stokes equations
 - Rotations and reflections
 - Scaling transformations
 - Etc.
- Assumptions
 - Symmetries apply to *filtered* Navier-Stokes equations
- Goal
 - Make model invariant
- Importance
 - Be able to represent solutions well

Symmetry requirements

- Condition of isotropy

$$Q_{\tau}^{mod} Q^T = f(Q\bar{S}Q^T, Q\bar{\Omega}Q^T)$$

- Orthogonal transformation of the coordinate frame: Q

- Importance

- Independence of observation angle

- Model constraint

- Coefficients depend on scalar quantities:

$$\alpha'_i = \alpha'_i(I_1, I_2, \dots, I_6)$$



$$\begin{array}{c} I_1 = \text{tr}(\bar{S}^2) \\ \dots \end{array}$$

Symmetry requirements

- Scaling symmetry

$$\begin{aligned} \hat{t} &= e^{2a} t & \hat{u}_i &= e^{-a+b} \hat{u}_i & \hat{v} &= e^{2b} v \\ \hat{x}_i &= e^{a+b} x_i & \hat{p} &= e^{-2a+2b} \bar{p} \end{aligned}$$

- Condition

$$\hat{\tau}^{mod} = e^{-2a+2b} \tau^{mod}$$

- Importance

- Represent self-similar solutions well

- Model constraint

- Units of the model coefficients, α'_i

Symmetry requirements

- Scaling symmetry constraint (I)

$$\begin{aligned}
 \underbrace{\tau^{mod}}_{m^2 s^{-2}} &= \underbrace{v_0}_{m^2 s^{-1}} \underbrace{f_0(I_1, I_2, \dots, I_6)}_{s^{-1}} \underbrace{I_1}_{1} \\
 &+ \underbrace{v_1}_{m^2 s^{-1}} \underbrace{f_1(I_1, I_2, \dots, I_6)}_{1} \underbrace{\bar{S}}_{s^{-1}} \\
 &+ \underbrace{v_2}_{m^2 s^{-1}} \underbrace{f_2(I_1, I_2, \dots, I_6)}_s \underbrace{(\bar{S}^2 - \dots)}_{s^{-2}} + \dots
 \end{aligned}$$

$$\begin{aligned}
 I_1 &= \text{tr}(\bar{S}^2) \\
 &\dots
 \end{aligned}$$

- Dependence of α'_i on I_1, I_2, \dots, I_6 partly determined
 - Units of f_i known
 - Limiting cases

Symmetry requirements

- Scaling symmetry constraint (II)

$$\begin{aligned}
 \underbrace{\tau^{mod}}_{m^2 s^{-2}} &= \underbrace{c_0}_{1} \underbrace{\delta^2}_{m^2} \underbrace{f_0(I_1, I_2, \dots, I_6)}_{s^{-2}} \underbrace{I_1}_{1} \\
 &+ \underbrace{c_1}_{1} \underbrace{\delta^2}_{m^2} \underbrace{f_1(I_1, I_2, \dots, I_6)}_{s^{-1}} \underbrace{\bar{S}}_{s^{-1}} \\
 &+ \underbrace{c_2}_{1} \underbrace{\delta^2}_{m^2} \underbrace{f_2(I_1, I_2, \dots, I_6)}_{1} \underbrace{(\bar{S}^2 - \dots)}_{s^{-2}} + \dots
 \end{aligned}$$

$$\begin{aligned}
 I_1 &= \text{tr}(\bar{S}^2) \\
 &\dots
 \end{aligned}$$

- Dependence of α'_i on I_1, I_2, \dots, I_6 partly determined
 - Units of f_i known
 - Limiting cases
- Requires dynamic procedure due to external length scale δ

The vanishing subgrid dissipation requirement

- Vreman's requirement for eddy viscosity models

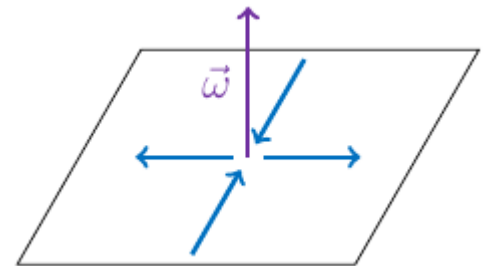
$$\text{tr}(\boldsymbol{\tau}\bar{\boldsymbol{S}}) = \boldsymbol{\tau} : \bar{\boldsymbol{S}} = 0 \rightarrow \text{tr}(\boldsymbol{\tau}^{mod}\bar{\boldsymbol{S}}) = 0$$

- Procedure

- Choose a certain flow / velocity gradient $\left[\frac{\partial u_i}{\partial x_j}\right]$, e.g. $\begin{bmatrix} 0 & 0 & * \\ 0 & 0 & * \\ 0 & 0 & 0 \end{bmatrix}$
- Compute $\boldsymbol{\tau}$ and $\bar{\boldsymbol{S}}$
- Compute subgrid dissipation $\text{tr}(\boldsymbol{\tau}\bar{\boldsymbol{S}})$
- If zero, require $\text{tr}(\boldsymbol{\tau}^{mod}\bar{\boldsymbol{S}}) = 0$

- Results

- Determines zeros of $\alpha'_1(I_1, I_2, \dots, I_6) = \text{tr}(\boldsymbol{\tau}^{mod}\bar{\boldsymbol{S}}) / I_1$



The vanishing subgrid force requirement

- Extending Vreman's requirement

$$-\frac{\partial}{\partial x_j} \tau_{ij} = 0 \rightarrow -\frac{\partial}{\partial x_j} \tau_{ij}^{mod} = 0$$

- Procedure

– Choose a certain flow / velocity gradient $\left[\frac{\partial u_i}{\partial x_j} \right]$, e.g. $\begin{bmatrix} 0 & 0 & * \\ 0 & 0 & * \\ 0 & 0 & 0 \end{bmatrix}$

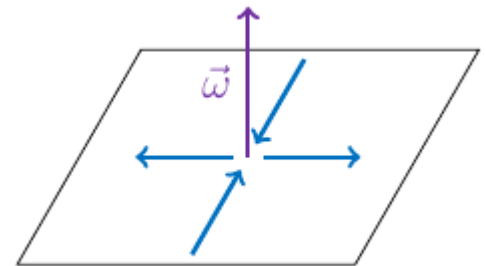
– Compute subgrid force $\frac{\partial}{\partial x_j} \tau_{ij}$

– If zero, require $\frac{\partial}{\partial x_j} \tau_{ij}^{mod} = 0$

- Results

– Determines zeros of $\alpha'_1(I_1, I_2, \dots, I_6)$

– Provides relation between $\alpha'_0, \alpha'_2, \alpha'_4$ for certain flows



Class of nonlinear models

- We have found a class of subgrid-scale models
 - nonlinear in \bar{S} and $\bar{\Omega}$
 - consisting of a finite number of independent terms
 - usually providing a representation of τ
 - satisfying several physical constraints
- We have discussed several physical model constraints
 - satisfying the symmetries of the Navier-Stokes equations:
 $\alpha'_i(I_1, I_2, \dots, I_6)$, with proper units
 - vanishing subgrid dissipation and subgrid force for simple flows:
zeros of α'_1 , relation between $\alpha'_0, \alpha'_2, \alpha'_4$

$$\tau^{mod} = \sum_{i=0}^7 \alpha'_i T'_i$$

Analysis of existing models

- Vreman's model

$$\boldsymbol{\tau}^{mod} - \frac{1}{3} \text{tr}(\boldsymbol{\tau}^{mod}) I = \alpha'_1 \bar{\boldsymbol{S}} \quad \alpha'_1 = -2c\delta^2 \sqrt{\frac{(I_1 - I_2)^2 - \frac{1}{2}(I_1 + I_2)^2 + 8I_5}{I_1 - I_2}}$$

- can only satisfy scale invariance if c is determined dynamically
- α'_1 vanishes when $\text{tr}(\boldsymbol{\tau}\bar{\boldsymbol{S}}) = 0$ ✓

- QR model

$$\boldsymbol{\tau}^{mod} - \frac{1}{3} \text{tr}(\boldsymbol{\tau}^{mod}) I = \alpha'_1 \bar{\boldsymbol{S}} \quad \alpha'_1 = -2C_\delta \frac{\max(0, I_3)}{I_1}$$

- can only satisfy scale invariance if C_δ is determined dynamically
- α'_1 vanishes for all two-dimensional strains ✗

Outlook

- Expectations of our class of subgrid-scale models
 - Better representation of subgrid-scale stresses than eddy viscosity models
 - Capture other than dissipative effects
- Future research
 - Discover which processes are represented by the different nonlinear model terms
 - Run flow simulations with different choices for the model coefficients satisfying the discussed constraints
- Any suggestions?
 - Additional physical constraints?
 - Interpretation of the nonlinear model terms?

Thank you for your attention!



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