Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows

Jens Lang

TECHNISCHE
UNIVERSITÄT
DARMSTADT

joint work with C. Hertel, J. Fröhlich (TU Dresden),
S. Löbig, M. Frankenbach, Z. Sun

Adaptive Numerical Methods
for Partial Differential Equations with Applications
Banff, May 28th to June 1st 2018

Overview

- Short introduction to large eddy simulation (LES)
- Motivation for using moving meshes
- Physically and mathematically based r-adaptation
- Turbulent flow over periodic hills
- Baroclinically unstable jet flow
- Stationary low Mach number combustion
- Summary

Incompressible Navier-Stokes-Equation

$$\begin{aligned}
\partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p - \nabla\cdot(2\nu\,\boldsymbol{S}(\boldsymbol{u})) &= \boldsymbol{f}, && \text{in } (0,T]\times\Omega \\
\nabla\cdot\boldsymbol{u} &= 0, && \text{in } (0,T]\times\Omega \\
\boldsymbol{u} &= \boldsymbol{u}_d, && \text{on } (0,T]\times\partial\Omega_D \\
p\boldsymbol{n} - 2\nu S(\boldsymbol{u})\boldsymbol{n} &= 0, && \text{on } (0,T]\times\partial\Omega^- \\
\boldsymbol{u} &= \boldsymbol{u}_0(\boldsymbol{x}), && \text{in } \{0\}\times\Omega
\end{aligned}$$

with $\Omega \in \mathbb{R}^3$ and $\boldsymbol{S}(\boldsymbol{u}) = (\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)/2$.

Incompressible Navier-Stokes-Equation

$$\begin{aligned}
\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla p - \nabla \cdot (2\nu\, \boldsymbol{S}(\boldsymbol{u})) &= \boldsymbol{f}, && \text{in } (0,T] \times \Omega \\
\nabla \cdot \boldsymbol{u} &= 0, && \text{in } (0,T] \times \Omega \\
\boldsymbol{u} &= \boldsymbol{u}_d, && \text{on } (0,T] \times \partial\Omega_D \\
p\boldsymbol{n} - 2\nu S(\boldsymbol{u})\boldsymbol{n} &= 0, && \text{on } (0,T] \times \partial\Omega^- \\
\boldsymbol{u} &= \boldsymbol{u}_0(\boldsymbol{x}), && \text{in } \{0\} \times \Omega
\end{aligned}$$

with $\Omega \in \mathbb{R}^3$ and $\boldsymbol{S}(\boldsymbol{u}) = (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)/2$.

Large Eddy Simulation (LES): Apply spatial filter to compute $\overline{\boldsymbol{u}} = G_\triangle \star u$.

Incompressible Navier-Stokes-Equation

$$\begin{aligned}
\partial_t \boldsymbol{u} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p - \nabla\cdot(2\nu\,\boldsymbol{S}(\boldsymbol{u})) &= \boldsymbol{f}, && \text{in } (0,T]\times\Omega \\
\nabla\cdot\boldsymbol{u} &= 0, && \text{in } (0,T]\times\Omega \\
\boldsymbol{u} &= \boldsymbol{u}_d, && \text{on } (0,T]\times\partial\Omega_D \\
p\boldsymbol{n} - 2\nu S(\boldsymbol{u})\boldsymbol{n} &= 0, && \text{on } (0,T]\times\partial\Omega^- \\
\boldsymbol{u} &= \boldsymbol{u}_0(\boldsymbol{x}), && \text{in } \{0\}\times\Omega
\end{aligned}$$

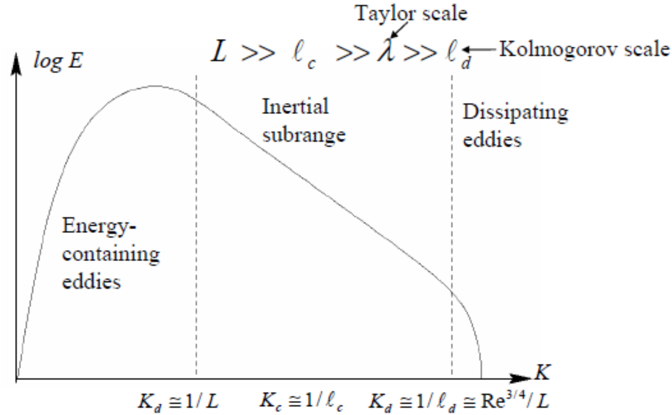
with $\Omega \in \mathbb{R}^3$ and $\boldsymbol{S}(\boldsymbol{u}) = (\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)/2$.

Large Eddy Simulation (LES): Apply spatial filter to compute $\overline{\boldsymbol{u}} = G_\triangle \star u$.

$$\begin{aligned}
\partial_t \overline{\boldsymbol{u}} + (\overline{\boldsymbol{u}}\cdot\nabla)\overline{\boldsymbol{u}} + \nabla\overline{p} - \nabla\cdot(2\nu S(\overline{\boldsymbol{u}})) &= \overline{\boldsymbol{f}} - \nabla\cdot\tau(\boldsymbol{u},\overline{\boldsymbol{u}}), && \text{in } (0,T]\times\Omega \\
\nabla\cdot\overline{\boldsymbol{u}} &= 0, && \text{in } (0,T]\times\Omega \\
\overline{\boldsymbol{u}} &= \overline{\boldsymbol{u}}_d, && \text{on } (0,T]\times\partial\Omega_D \\
\overline{p}\boldsymbol{n} - 2\nu S(\overline{\boldsymbol{u}})\boldsymbol{n} &= 0, && \text{on } (0,T]\times\partial\Omega^- \\
\overline{\boldsymbol{u}} &= \overline{\boldsymbol{u}}_0(\boldsymbol{x}), && \text{in } \{0\}\times\Omega
\end{aligned}$$

where the stress tensor $\tau(\boldsymbol{u},\overline{\boldsymbol{u}}) = \overline{\boldsymbol{u}\,\boldsymbol{u}} - \overline{\boldsymbol{u}}\,\overline{\boldsymbol{u}}$ has to be modelled.

Large Eddy Simulation



Goal: LES models the smallest (and most expensive) scales and resolves large scales of the flow field solution.

Miracle: Turbulent Motion of Fluids

Werner Heisenberg was asked what he would ask God, given the opportunity. His reply was:

When I meet God, I am going to ask him two questions: Why relativity? And why turbulence? I really believe he will have an answer for the first.

Miracle: Turbulent Motion of Fluids

Werner Heisenberg was asked what he would ask God, given the opportunity. His reply was:

When I meet God, I am going to ask him two questions: Why relativity? <u>And why turbulence?</u> I really believe he will have an answer for the first.

Horace Lamb (who had published a noted text book on Hydrodynamics) was quoted as saying

I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is <u>the turbulent motion of fluids</u>. And about the former I am rather optimistic.

Filtered Incompressible Navier-Stokes-Equation

Use eddy viscosity model (Smagorinsky model)

$$\tau(\boldsymbol{u}, \overline{\boldsymbol{u}}) \approx \tau_s(\overline{\boldsymbol{u}}) \;=\; -\nu_t(\overline{\boldsymbol{u}})\, S(\overline{\boldsymbol{u}})$$

with turbulent viscosity defined by

$$\nu_t(\overline{\boldsymbol{u}}) \;=\; (c_s \triangle)^2 \sqrt{2} ||S(\overline{\boldsymbol{u}})||, \quad ||S(\overline{\boldsymbol{u}})|| \;=\; (S(\overline{\boldsymbol{u}}) : S(\overline{\boldsymbol{u}}))^{1/2}$$

Filtered Incompressible Navier-Stokes-Equation

Use eddy viscosity model (Smagorinsky model)

$$\tau(\boldsymbol{u}, \overline{\boldsymbol{u}}) \approx \tau_s(\overline{\boldsymbol{u}}) \;=\; -\nu_t(\overline{\boldsymbol{u}})\, S(\overline{\boldsymbol{u}})$$

with turbulent viscosity defined by

$$\nu_t(\overline{\boldsymbol{u}}) \;=\; (c_s \triangle)^2 \sqrt{2} ||S(\overline{\boldsymbol{u}})||, \quad ||S(\overline{\boldsymbol{u}})|| \;=\; \left(S(\overline{\boldsymbol{u}}) : S(\overline{\boldsymbol{u}})\right)^{1/2}$$

Smagorinsky constant: $c_s = 0.1 - 0.2$, dynamic Smagorinsky $c_s = c_s(\overline{\boldsymbol{u}})$

Filtered Incompressible Navier-Stokes-Equation

Use eddy viscosity model (Smagorinsky model)

$$\tau(\boldsymbol{u}, \overline{\boldsymbol{u}}) \approx \tau_s(\overline{\boldsymbol{u}}) \;=\; -\nu_t(\overline{\boldsymbol{u}})\, S(\overline{\boldsymbol{u}})$$

with turbulent viscosity defined by

$$\nu_t(\overline{\boldsymbol{u}}) \;=\; (c_s \triangle)^2 \sqrt{2} ||S(\overline{\boldsymbol{u}})||, \quad ||S(\overline{\boldsymbol{u}})|| \;=\; (S(\overline{\boldsymbol{u}}) : S(\overline{\boldsymbol{u}}))^{1/2}$$

Smagorinsky constant: $c_s = 0.1 - 0.2$, dynamic Smagorinsky $c_s = c_s(\overline{\boldsymbol{u}})$

Closed model for $(\overline{\boldsymbol{u}}_s, \overline{p}_s)$:

$$\begin{array}{rcll} \partial_t \overline{\boldsymbol{u}}_s + (\overline{\boldsymbol{u}}_s \cdot \nabla)\overline{\boldsymbol{u}}_s + \nabla \overline{p}_s - \nabla \cdot ((2\nu + \nu_t) S(\overline{\boldsymbol{u}}_s)) & = & \overline{\boldsymbol{f}}, & (0, T] \times \Omega \\ \nabla \cdot \overline{\boldsymbol{u}}_s & = & 0, & (0, T] \times \Omega \\ \overline{\boldsymbol{u}}_s & = & \overline{\boldsymbol{u}}_d, & (0, T] \times \partial\Omega_D \\ \overline{p}_s \boldsymbol{n} - (2\nu + \nu_t) S(\overline{\boldsymbol{u}}_s)\boldsymbol{n} & = & 0, & (0, T] \times \partial\Omega^- \\ \overline{\boldsymbol{u}}_s & = & \overline{\boldsymbol{u}}_0(\boldsymbol{x}), & \{0\} \times \Omega \end{array}$$

Errors in Large Eddy Simulation

Good news: Nowadays LES works quite well provided

- sufficient computer resources are available,
- advanced knowledge on physics and numerical methods.

Errors in Large Eddy Simulation

Good news: Nowadays LES works quite well provided

- sufficient computer resources are available,
- advanced knowledge on physics and numerical methods.

Two main error sources:

- Filtering, sgs, b.c. give rise to modelling errors.
- Numerical schemes give rise to discretization errors.

Errors in Large Eddy Simulation

Good news: Nowadays LES works quite well provided

- sufficient computer resources are available,
- advanced knowledge on physics and numerical methods.

Two main error sources:

- Filtering, sgs, b.c. give rise to modelling errors.
- Numerical schemes give rise to discretization errors.

Bad news: If $\Delta = h$ (most practical) is used then modelling and discretization errors interact.

Errors in Large Eddy Simulation

Good news: Nowadays LES works quite well provided

- sufficient computer resources are available,
- advanced knowledge on physics and numerical methods.

Two main error sources:

- Filtering, sgs, b.c. give rise to modelling errors.
- Numerical schemes give rise to discretization errors.

Bad news: If $\Delta = h$ (most practical) is used then modelling and discretization errors interact.

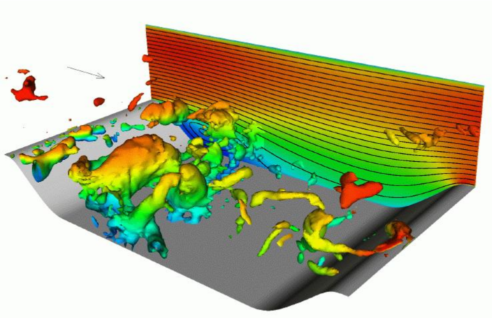
Need for a posteriori quality improvement of LES!

LES - Statistics

- LES produces huge data of space- and time-resolved flow solutions, but often one is only interested in statistical values as mean velocities and fluctuations, which can be compared to experimental data.

LES - Statistics

- LES produces huge data of space- and time-resolved flow solutions, but often one is only interested in statistical values as mean velocities and fluctuations, which can be compared to experimental data.



LES for flow over periodic hills, $Re = 10595$.

LES - Statistics

- Define time-averaging

$$\langle \boldsymbol{v} \rangle(\mathbf{x}) = \lim_{T\to\infty} \frac{1}{T} \int_0^T \boldsymbol{v}(t, \mathbf{x})\, dt$$

and fluctuations

$$\boldsymbol{v}'' = \boldsymbol{v} - \langle \boldsymbol{v} \rangle$$

LES - Statistics

- Define time-averaging

$$\langle \boldsymbol{v} \rangle(\mathbf{x}) = \lim_{T \to \infty} \frac{1}{T} \int_0^T \boldsymbol{v}(t, \mathbf{x})\, dt$$

  and fluctuations

$$\boldsymbol{v}'' = \boldsymbol{v} - \langle \boldsymbol{v} \rangle$$

- For LES it holds

$$\langle \overline{\boldsymbol{u}}''\, \overline{\boldsymbol{u}}'' \rangle \approx \langle \tau(\boldsymbol{u}, \overline{\boldsymbol{u}}) \rangle + \langle \overline{\boldsymbol{u}}\, \overline{\boldsymbol{u}} \rangle - \langle \overline{\boldsymbol{u}} \rangle \langle \overline{\boldsymbol{u}} \rangle \,,$$

  which gives a possibility to approximate the time-averaged stress tensor $\langle \tau(\boldsymbol{u}, \overline{\boldsymbol{u}}) \rangle$.

Motivation for Mesh Adaptation

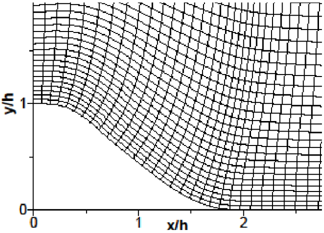
- Multi-scale modelling with variable filter width $\triangle = h(\overline{\boldsymbol{u}}_s)$ yields resolved subgrid-scale turbulence.

Motivation for Mesh Adaptation

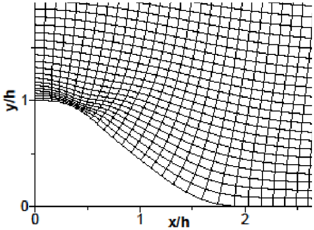
- Multi-scale modelling with variable filter width $\triangle = h(\overline{\boldsymbol{u}}_s)$ yields resolved subgrid-scale turbulence.
- Optimizing LES via r-adaption (redistribution=moving mesh)
- Appropriate monitor functions for LES

Motivation for Mesh Adaptation

- Multi-scale modelling with variable filter width $\triangle = h(\overline{\boldsymbol{u}}_s)$ yields resolved subgrid-scale turbulence.
- Optimizing LES via r-adaption (redistribution=moving mesh)
- Appropriate monitor functions for LES
- Adaptive scale separation w.r.t. time-averaged solution



$\Longrightarrow$



Mesh Moving Method

- Physical domain Ω with coordinates $\mathbf{x} = (x_1, x_2, x_3)^T$
- Computational domain Ω_c with coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$

Mesh Moving Method

- Physical domain Ω with coordinates $\mathbf{x} = (x_1, x_2, x_3)^T$
- Computational domain Ω_c with coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$
- Solution of the physical PDE: $(\overline{\boldsymbol{u}}_s, \overline{p}_s) = (\overline{\boldsymbol{u}}_s, \overline{p}_s)(\mathbf{x}, t)$
- 1-1 coordinate transformation $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi}, t)$

Mesh Moving Method

- Physical domain Ω with coordinates $\mathbf{x} = (x_1, x_2, x_3)^T$
- Computational domain Ω_c with coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$
- Solution of the physical PDE: $(\overline{\boldsymbol{u}}_s, \overline{p}_s) = (\overline{\boldsymbol{u}}_s, \overline{p}_s)(\mathbf{x}, t)$
- 1-1 coordinate transformation $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi}, t)$
- Minimise mesh adaptation functional (equidistribution principle)

$$\mathcal{I}[\boldsymbol{\xi}] = \frac{1}{2} \int_\Omega \sqrt{g} \sum_{i=1}^{3} \nabla\xi_i \, G^{-1} \, \nabla\xi_i \, d\boldsymbol{x}, \quad g = \det(G)$$

Mesh Moving Method

- Physical domain Ω with coordinates $\mathbf{x} = (x_1, x_2, x_3)^T$
- Computational domain Ω_c with coordinates $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$
- Solution of the physical PDE: $(\overline{\boldsymbol{u}}_s, \overline{p}_s) = (\overline{\boldsymbol{u}}_s, \overline{p}_s)(\mathbf{x}, t)$
- 1-1 coordinate transformation $\mathbf{x} = \mathbf{x}(\boldsymbol{\xi}, t)$
- Minimise mesh adaptation functional (equidistribution principle)

$$\mathcal{I}[\boldsymbol{\xi}] = \frac{1}{2} \int_{\Omega} \sqrt{g} \sum_{i=1}^{3} \nabla \xi_i \, G^{-1} \, \nabla \xi_i \, d\boldsymbol{x}, \quad g = \det(G)$$

- Derive time-dependent mesh moving PDE

Mesh Moving Method

Time-dependent Mesh Moving PDE [Huang, Russell]:

$$\tau \frac{\partial \boldsymbol{x}}{\partial t} = \frac{1}{P} \left(\sum_{i,j} a_{ij} \frac{\partial^2 \boldsymbol{x}}{\partial \xi_i \partial \xi_j} - \sum_i b_i \frac{\partial \boldsymbol{x}}{\partial \xi_i} \right)$$

where

$$a_{ij} = \nabla \xi_i \cdot G^{-1} \nabla \xi_j, \quad b_i = \sum_j \nabla \xi_i \cdot \frac{\partial G^{-1}}{\partial \xi_j} \nabla \xi_j, \quad P^2 = \sum_{i,j} a_{ij}^2 + \sum_i b_i^2$$

Mesh Moving Method

Time-dependent Mesh Moving PDE [Huang, Russell]:

$$\tau \frac{\partial \boldsymbol{x}}{\partial t} = \frac{1}{P} \left(\sum_{i,j} a_{ij} \frac{\partial^2 \boldsymbol{x}}{\partial \xi_i \partial \xi_j} - \sum_i b_i \frac{\partial \boldsymbol{x}}{\partial \xi_i} \right)$$

where

$$a_{ij} = \nabla \xi_i \cdot G^{-1} \nabla \xi_j, \quad b_i = \sum_j \nabla \xi_i \cdot \frac{\partial G^{-1}}{\partial \xi_j} \nabla \xi_j, \quad P^2 = \sum_{i,j} a_{ij}^2 + \sum_i b_i^2$$

How to choose $G \in \mathbb{R}^{3\times 3}$?

Mesh Moving Method

Time-dependent Mesh Moving PDE [Huang, Russell]:

$$\tau \frac{\partial \mathbf{x}}{\partial t} = \frac{1}{P}\left(\sum_{i,j} a_{ij} \frac{\partial^2 \mathbf{x}}{\partial \xi_i \partial \xi_j} - \sum_i b_i \frac{\partial \mathbf{x}}{\partial \xi_i} \right)$$

where

$$a_{ij} = \nabla \xi_i \cdot G^{-1} \nabla \xi_j, \quad b_i = \sum_j \nabla \xi_i \cdot \frac{\partial G^{-1}}{\partial \xi_j} \nabla \xi_j, \quad P^2 = \sum_{i,j} a_{ij}^2 + \sum_i b_i^2$$

How to choose $G \in \mathbb{R}^{3\times 3}$? Typical choice: $G = w(\Psi) I$.

Mesh Moving Method

Time-dependent Mesh Moving PDE [Huang, Russell]:

$$\tau \frac{\partial \boldsymbol{x}}{\partial t} = \frac{1}{P} \left(\sum_{i,j} a_{ij} \frac{\partial^2 \boldsymbol{x}}{\partial \xi_i \partial \xi_j} - \sum_i b_i \frac{\partial \boldsymbol{x}}{\partial \xi_i} \right)$$

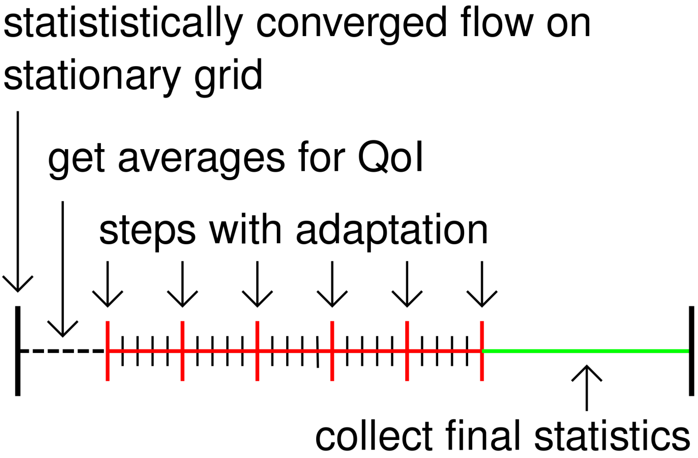
where

$$a_{ij} = \nabla \xi_i \cdot G^{-1} \nabla \xi_j, \quad b_i = \sum_j \nabla \xi_i \cdot \frac{\partial G^{-1}}{\partial \xi_j} \nabla \xi_j, \quad P^2 = \sum_{i,j} a_{ij}^2 + \sum_i b_i^2$$

How to choose $G \in \mathbb{R}^{3\times 3}$? Typical choice: $G = w(\Psi) I$.

Monitor function should depend on some quantity of interest Ψ, physically or mathematically motivated.

LES with Moving Meshes: General Strategy



Mesh Moving Method - Implementation

- Use LESOCC2 - advanced parallel code for engineering applications
- Second order cell-centered finite volume method for curvilinear coordinates, coupled with predictor-corrector scheme based on three-stage Runge-Kutta methods and pressure correction equation

Mesh Moving Method - Implementation

- Use LESOCC2 - advanced parallel code for engineering applications
- Second order cell-centered finite volume method for curvilinear coordinates, coupled with predictor-corrector scheme based on three-stage Runge-Kutta methods and pressure correction equation
- Implement arbitrary Lagrangian-Eulerian formulation (ALE) with time-varying control volumes $V(t)$ and surfaces $S(t)$

Mesh Moving Method - Implementation

- Use LESOCC2 - advanced parallel code for engineering applications
- Second order cell-centered finite volume method for curvilinear coordinates, coupled with predictor-corrector scheme based on three-stage Runge-Kutta methods and pressure correction equation
- Implement arbitrary Lagrangian-Eulerian formulation (ALE) with time-varying control volumes $V(t)$ and surfaces $S(t)$
- Ensure mass conservation via space conservation law [Demirdzic, Peric]

$$\frac{d}{dt}\int_{V(t)} dv - \int_{S(t)} u_N \boldsymbol{n}\, ds = 0$$

  where u_N is the (given) vector of node velocities. Adapt mesh movement.

Mesh Moving Method - Implementation
Cell Centered Finite Volume Method

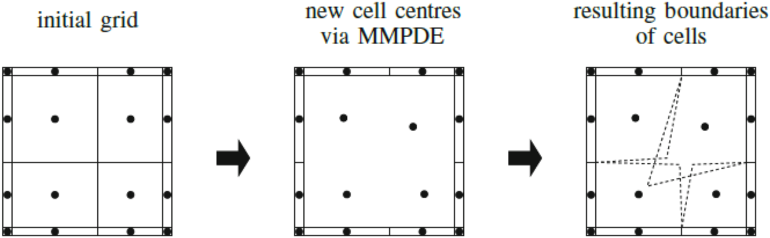


Illustration of difficulties when constructing a valid grid from cell centres

Mesh Moving Method - Implementation Cell Centered Finite Volume Method

Step 1 Integration of the MMPDE for cell centres with fixed points at boundaries yielding preliminary values of cell centres $\mathbf{x}^*$.

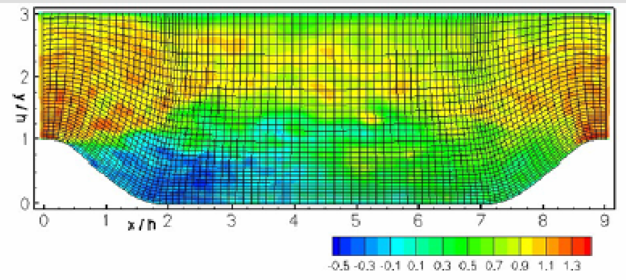
Step 2 Determination of cell corner points $\tilde{\mathbf{x}}^{\mathbf{n}+1}$ via an interpolation method.

Step 3 Determination of corner points on boundaries from final corner grid in the interior.

Step 4 Re-computation of cell centres $\mathbf{x}^{\mathbf{n}+1}$ in the domain and on the boundary to generate the final valid grid.

Hertel, Schümichen, JL, Fröhlich: *Using a Moving Mesh PDE for Cell Centres to Adapt a Finite Volume Grid*, Flow, Turbulence and Combustion 90(4), pp. 785–812, 2013.

Turbulent Flows over Periodic Hills



- $Re = 10595$
- Smagorinsky subgrid-scale model with $c_s = 0.1$
- Reference solution with 4.500.000 cells [Fröhlich et al., 2005]
- Computational grid: $89 \times 33 \times 49$ (135.168 cells)

The Engineer's Approach

Quantity of Interest Φ

Here: $\langle \cdot \rangle$ denotes averaging in homogeneous direction and time.

- Gradient of streamwise velocity: $\Phi = \nabla \langle \overline{\boldsymbol{u}}_1 \rangle$
- Modelled turbulent kinetic energy (TKE)

$$\Phi = \frac{\langle k_{sgs} \rangle}{k_{tot,max}}, \quad k_{sgs} \approx (2^{1/3} - 1) 0.5 |\overline{\boldsymbol{u}} - \overline{\overline{\boldsymbol{u}}}| \quad \text{[Berselli et al., 2006]}$$

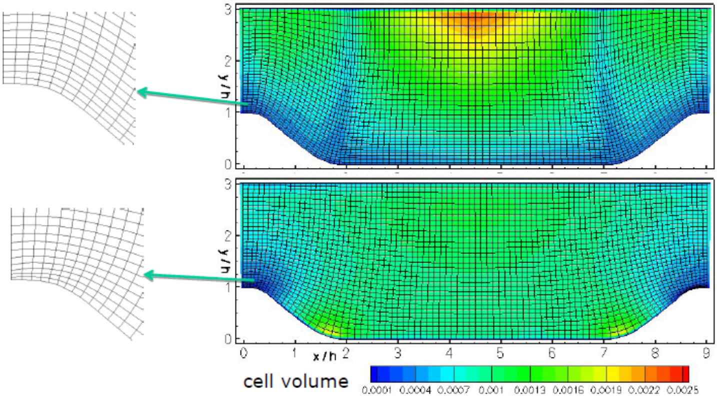
- Turbulent shear stress: ratio of modelled and total shear stress

$$\Phi = \frac{\langle \tau_{12}^{mod} \rangle}{\langle \tau_{12}^{mod} \rangle + \langle \overline{\boldsymbol{u}}_1'' \overline{\boldsymbol{u}}_2'' \rangle}, \quad \tau_{12}^{mod} = -\nu_t \left(\frac{\partial \overline{\boldsymbol{u}}_1}{\partial x_2} + \frac{\partial \overline{\boldsymbol{u}}_2}{\partial x_1} \right)$$

Use combination of them as well.

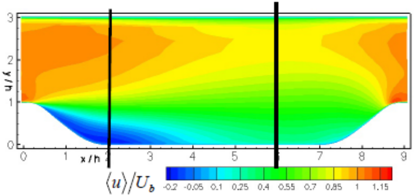
The Engineer's Approach

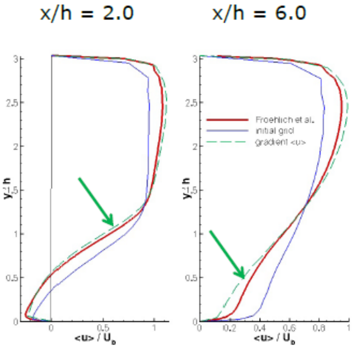
Monitor function: gradient of streamwise velocity $\Phi = \nabla \langle \overline{\boldsymbol{u}}_1 \rangle$



The Engineer's Approach

Monitor function: gradient of streamwise velocity $\Phi = \nabla \langle \overline{\boldsymbol{u}}_1 \rangle$



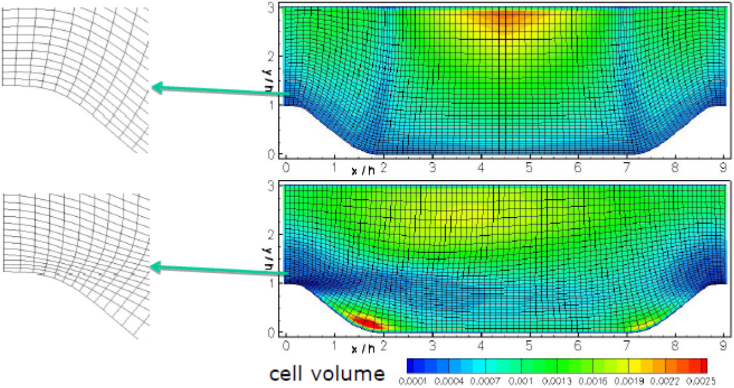


	x_{sep}/h	x_{rea}/h
Reference	0.2	4.6
Initial grid	0.5	3.1
with adaptation	0.3	4.7

Comparison of low separation and reattachment point

The Engineer's Approach

Monitor function: combine gradient of streamwise velocity and modelled kinetic energy $\Phi = \nabla\langle\overline{\boldsymbol{u}}_1\rangle + \frac{\langle k_{sgs}\rangle}{k_{tot,max}}$



The Engineer's Approach

Comparison of low separation and reattachment point

	x_{sep} /h	x_{rea} /h
Reference (5 Mio. cells)	0.2	4.6
Initial grid	0.5	3.1
1. $\nabla\langle u\rangle$	0.3	4.7
2. $\langle k_{sgs}\rangle / k_{tot,max}$	0.45	3.4
3. $\langle\tau_{12}^{mod}\rangle / \left(\langle\tau_{12}^{mod}\rangle + \langle u'v'\rangle\right)$	0.45	4.15
4. $\psi_1 = \nabla\langle u\rangle$ & $\psi_2 = \langle k_{sgs}\rangle / k_{tot,max}$	0.3	4.5
5. $\psi_1 = \nabla\langle u\rangle$ & $\psi_2 = \frac{\langle\tau_{12}^{mod}\rangle}{\langle\tau_{12}^{mod}\rangle + \langle u'v'\rangle}$	0.25	4.55

← **best**

The Mathematician's Approach

Dual Weighted Residual Method [Becker, Rannacher, Braack, ...]

The Mathematician's Approach

Dual Weighted Residual Method [Becker, Rannacher, Braack, ...]

Goal: quantify the contributions of the subgrid-scale model and the numerical method to a user specified quantity of interest

$$M(\langle \mathbf{u} \rangle, \langle p \rangle) = \int_\Omega N(\langle \mathbf{u} \rangle, \langle p \rangle) d\mathbf{x}$$

The Mathematician's Approach

Dual Weighted Residual Method [Becker, Rannacher, Braack, ...]

Goal: quantify the contributions of the subgrid-scale model and the numerical method to a user specified quantity of interest

$$M(\langle \mathbf{u} \rangle, \langle p \rangle) = \int_\Omega N(\langle \mathbf{u} \rangle, \langle p \rangle) d\mathbf{x}$$

Linearize N in the neighbourhood of $(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle)$:

$$M(\langle \mathbf{u} \rangle, \langle p \rangle) - M(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \quad =$$

$$\int_\Omega \left\{ \partial_{\langle \mathbf{u} \rangle} N(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \, \mathbf{e}_{\langle \mathbf{u} \rangle} + \partial_{\langle p \rangle} N(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \, \mathbf{e}_{\langle p \rangle} \right\} d\mathbf{x} + H.O.T.$$

with $\mathbf{e}_{\langle \mathbf{u} \rangle} = \langle \mathbf{u} \rangle - \langle \bar{\mathbf{u}}_h \rangle$ and $e_{\langle p \rangle} = \langle p \rangle - \langle \bar{p}_h \rangle$.

The Mathematician's Approach

Define (linear) stationary dual system with (ϕ, θ):

$$\begin{aligned} -(\langle \bar{\mathbf{u}}_h \rangle \cdot \nabla)\boldsymbol{\varphi} + (\nabla \langle \bar{\mathbf{u}}_h \rangle)^T \boldsymbol{\varphi} + \nabla\theta & \\ -\nabla \cdot ((2\nu + \nu_t(\langle \bar{\mathbf{u}}_h \rangle))S(\boldsymbol{\varphi})) - \nabla \cdot T^h[\langle \bar{\mathbf{u}}_h \rangle](\boldsymbol{\varphi}) &= \partial_{\langle \mathbf{u} \rangle} N(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \\ -\nabla \cdot \boldsymbol{\varphi} &= \partial_{\langle p \rangle} N(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \\ \boldsymbol{\varphi} &= 0 \qquad \text{b.c.} \\ \boldsymbol{\varphi}(T, \boldsymbol{x}) &= 0 \qquad \text{i.c.} \end{aligned}$$

where $T^h[\langle \bar{\mathbf{u}}_h \rangle](\varphi) = (c_s\, \Delta)^2 \, ||S(\langle \bar{\mathbf{u}}_h \rangle)||_F^{-1} (S(\langle \bar{\mathbf{u}}_h \rangle) : S(\varphi)) S(\langle \bar{\mathbf{u}}_h \rangle)$.

The Mathematician's Approach

Theorem [Computable error representation formula]
Let $(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle)$ be the numerical solution and N a given operator. Then

$$M(\langle \mathbf{u} \rangle, \langle p \rangle) - M(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \approx e_M + e_N + H.O.T.$$

The Mathematician's Approach

Theorem [Computable error representation formula]
Let $(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle)$ be the numerical solution and N a given operator. Then

$$M(\langle \mathbf{u} \rangle, \langle p \rangle) - M(\langle \bar{\mathbf{u}}_h \rangle, \langle \bar{p}_h \rangle) \approx e_M + e_N + H.O.T.$$

with e_M and e_N are given by

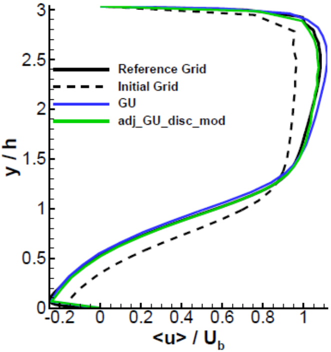
$$e_M = \int_\Omega \phi_h \left\{ \langle \mathbf{f} \rangle - \langle \bar{\mathbf{f}} \rangle + \langle (\nabla \cdot \tau_s)(\bar{\mathbf{u}}_h) \rangle - \langle \nabla \cdot \tau_{ds}(\bar{\mathbf{u}}_h) \rangle \right\} d\mathbf{x}$$

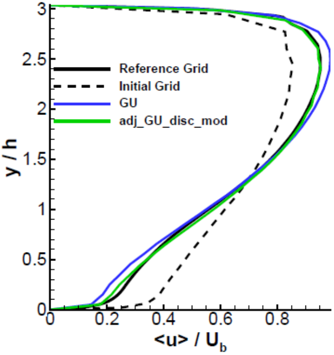
$$e_N = \int_\Omega \{ \phi_h \langle ResSM(\bar{\mathbf{u}}_h, \bar{p}_h) \rangle + \theta_h \langle \nabla \cdot \bar{\mathbf{u}}_h \rangle \} d\mathbf{x}$$

where $ResSM(\bar{\mathbf{u}}_h, \bar{p}_h)$ is the residual of the space-averaged momentum equation with Smagorinsky subgrid-scale model.

The Mathematician's Approach

Monitor function: $\Phi = \Phi_N + \Phi_M$ based on $N(\overline{\boldsymbol{u}}) = \nabla\langle\overline{\boldsymbol{u}}_1\rangle$

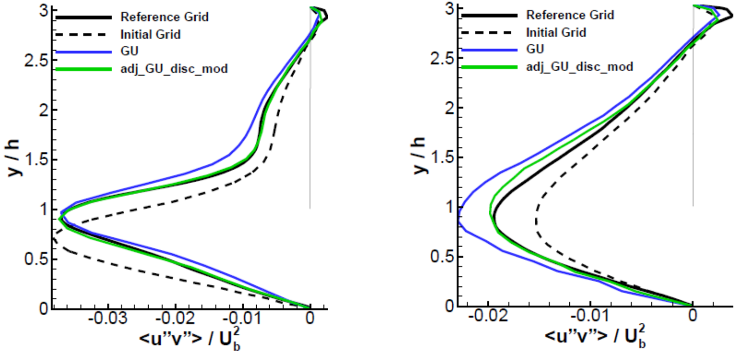




Comparison of $\nabla\langle\overline{\boldsymbol{u}}_1\rangle/U_b$ at $x/h = 2$ and $x/h = 6$.

The Mathematician's Approach

Monitor function: $\Phi = \Phi_N + \Phi_M$ based on $N(\overline{\boldsymbol{u}}) = \nabla\langle\overline{\boldsymbol{u}}_1\rangle$



Comparison of $\langle\overline{\boldsymbol{u}}_1''\overline{\boldsymbol{u}}_2''\rangle/U_b^2$ at $x/h = 2$ and $x/h = 6$.

Meteorological Application

German Priority Program 'METSTROEM' (Funded by DFG)

Collaborators in the first period: C. Kühnlein, A. Dörnbrack (Munich), P.K. Smolarkiewicz (Boulder)

Software Package MPDATA and EULAG

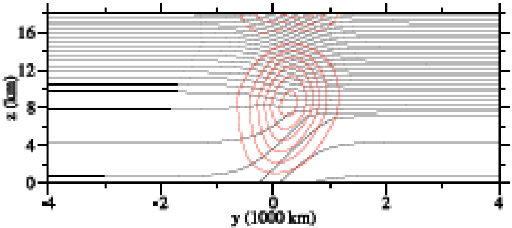
Meteorological Application

German Priority Program 'METSTROEM' (Funded by DFG)

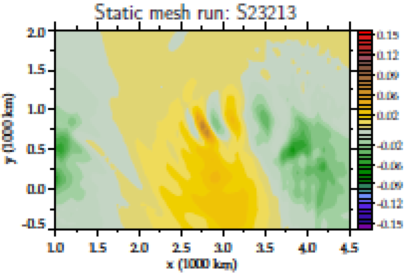
Collaborators in the first period: C. Kühnlein, A. Dörnbrack (Munich), P.K. Smolarkiewicz (Boulder)

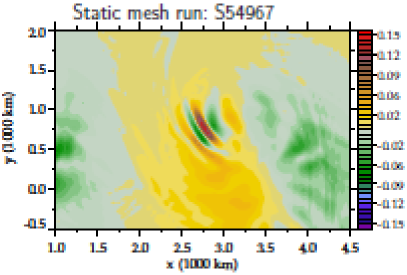
Software Package MPDATA and EULAG

Application:
Baroclinically unstable jet flow in inviscid and dry atmosphere
Zonally-periodic channel: 10.000 km $\times$ 8.000 km $\times$ 18 km



Meteorological Application: Baroclinically Unstable Jet Flow in Inviscid and Dry Atmosphere



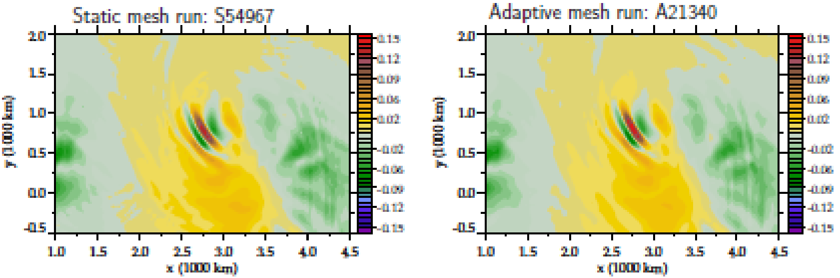


Representation of mesoscale internal gravity waves

$$\Phi = 1/H \int_0^H \|\nabla \Theta(t, x, y, z)\| \, dz$$

(C. Kühnlein, A. Dörnbrack, P.K. Smolarkiewicz, 2011)

Meteorological Application: Baroclinically Unstable Jet Flow in Inviscid and Dry Atmosphere



Representation of mesoscale internal gravity waves

$$\Phi = 1/H \int_0^H \|\nabla\Theta(t,x,y,z)\|\, dz$$

(C. Kühnlein, A. Dörnbrack, P.K. Smolarkiewicz, 2011)

Low Mach Number Compressible Combustion

$$
\begin{aligned}
\rho\partial_t \boldsymbol{u} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} + \nabla p_{hyd} - \nabla\cdot(2\nu\,\boldsymbol{S}(\boldsymbol{u})) &= \rho\boldsymbol{g}, && \text{in } (0,T]\times\Omega \\
\frac{1}{M}\boldsymbol{u}\cdot\nabla M - \frac{1}{T}\boldsymbol{u}\cdot\nabla T + \nabla\cdot\boldsymbol{u} &= 0, && \text{in } (0,T]\times\Omega \\
c_p\partial_t T + c_p\rho\boldsymbol{u}\cdot\nabla T - \nabla\cdot(\lambda\nabla T) &= f_T(T,\boldsymbol{\omega}), && \text{in } (0,T]\times\Omega \\
\partial_t\omega_i + \rho\boldsymbol{u}\cdot\nabla\omega_i - \nabla\cdot(\rho D_i\nabla\omega_i) &= f_i(T,\boldsymbol{\omega}), && \text{in } (0,T]\times\Omega \\
& \quad i = 1:N, && \Omega\subset\mathbb{R}^2
\end{aligned}
$$

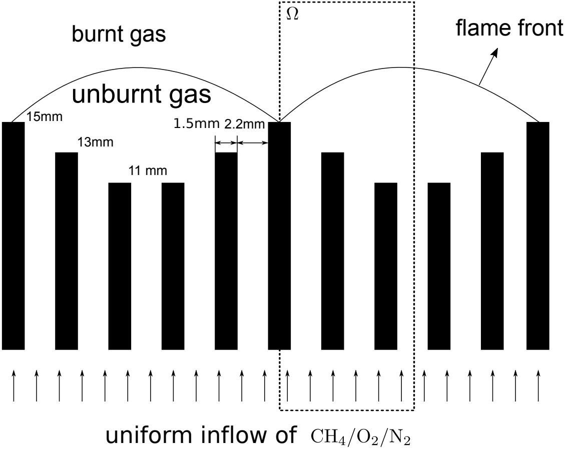
$$
\rho = \frac{P_{th}M}{RT}, \quad \frac{1}{M} = \sum_{i=1}^{N}\frac{\omega_i}{M_i}
$$

Methane Burner (JUNKERS Bosch Thermotechnik, 1988) with global reaction

$$
CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O
$$

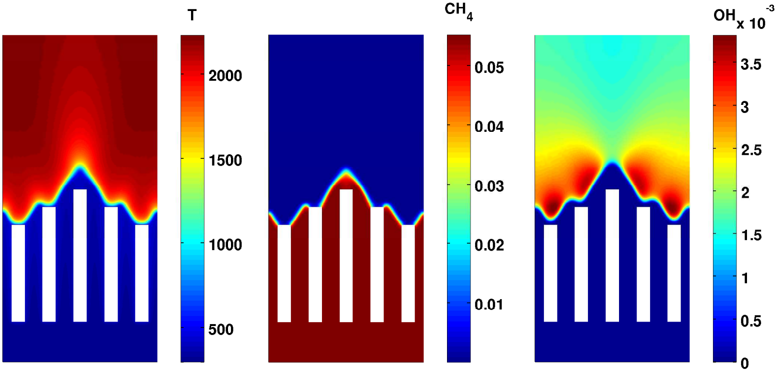
$N = 15$ species and 84 elementary reactions (no NO_x formation)

Methane Burner



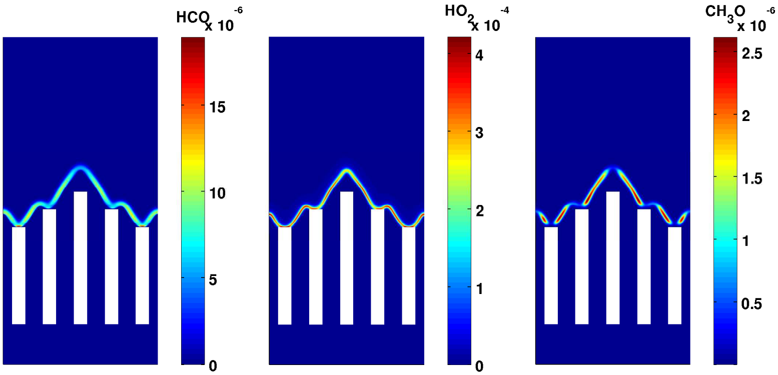
Geometry of the Junkers Bosch Methane Burner

Methane Burner



Stationary solutions: T, CH_4, and OH

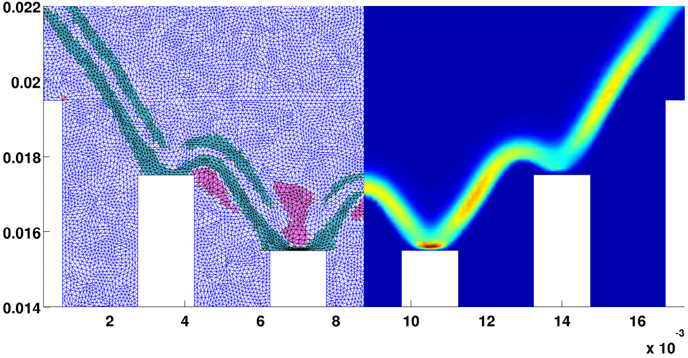
Methane Burner



Stationary solutions: HCO (Hydrocarbonate), HO_2, and CH_3O

Moving Meshes for the Methane Burner

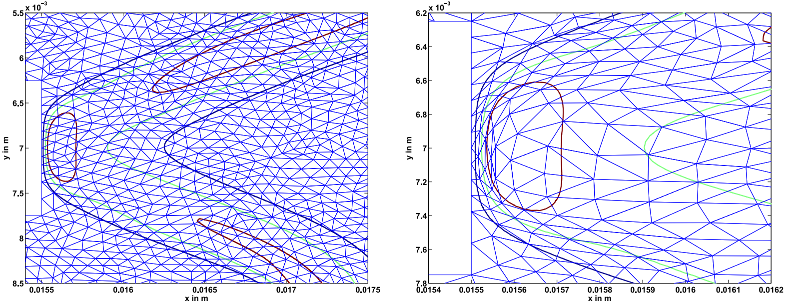
Quantity of Interest: $\Phi = \nabla \omega_{CHO}$



Profile of radical HCO. The elements in magenta represent enlarged triangles (rate: +0.15), and the cyan ones show the compressed cells (rate: -0.05).

Moving Meshes for the Methane Burner

Quantity of Interest: $\Phi = \nabla \omega_{CHO}$



Initial mesh (left) and adaptive mesh (right) close to the shortest slot.

Summary

- LES is well suited for moving mesh techniques.
- Physically motivated monior functions work quite well for LES.
- High potential of sensitivity-based mesh moving methods based on adaptive scale separation.
- Resolve as much physics as possible with given DoFs: Model dissipation and resolve production.
- Application of moving meshes to complex combustion still needs expert knowledge.

Final Remark

Independent (UK), 4th May 2018
Karl Marx 200th anniversary

The world is finally ready for Marxism as capitalism reaches the tipping point.

Final Remark

Independent (UK), 4th May 2018
Karl Marx 200th anniversary

The world is finally ready for Marxism as capitalism reaches the tipping point.

The world is finally ready for Moving Meshes as uniform ones reach the tipping point.

Banff, 31st May 2018

Final Remark

Independent (UK), 4th May 2018
Karl Marx 200th anniversary

The world is finally ready for Marxism as capitalism reaches the tipping point.

The world is finally ready for Moving Meshes as uniform ones reach the tipping point.

Banff, 31st May 2018