UNSTEADY FLOW MODELLING AND COMPUTATION

Franck Nicoud

University Montpellier II – I3M CNRS UMR 5149

and

CERFACS

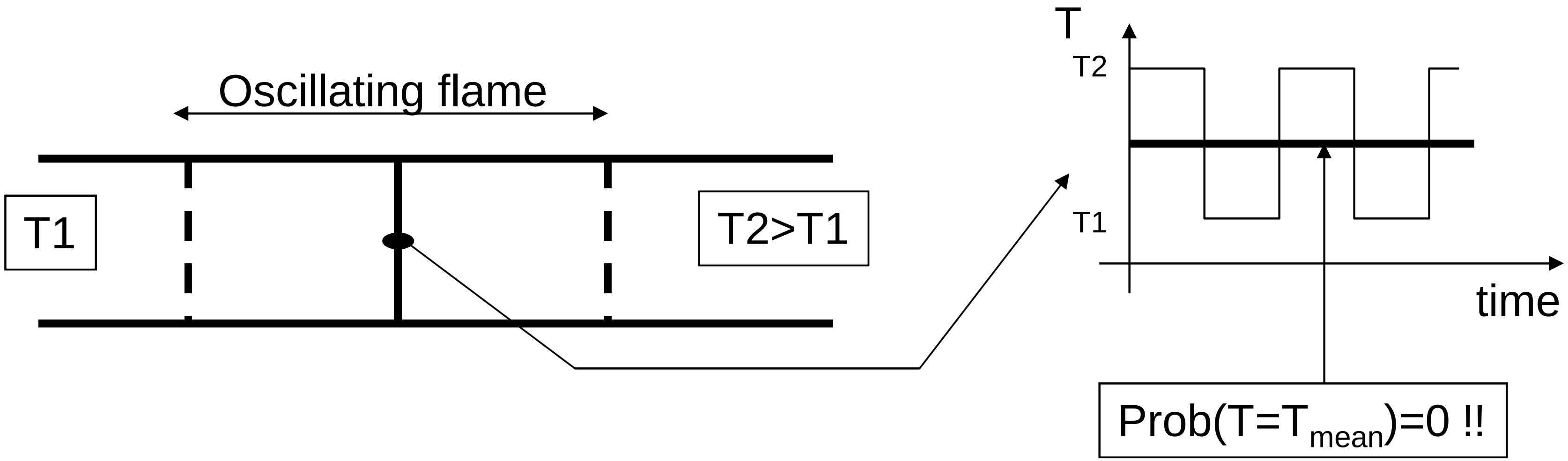
MOTIVATION - 1

- CFD of steady flow is now mature
- Many industrial codes available, robust and accurate
- Complex flow physics included: moving geometries, turbulence, combustion, mixing, fluid-X coupling
- But only the averages are computed

MOTIVATION - 2

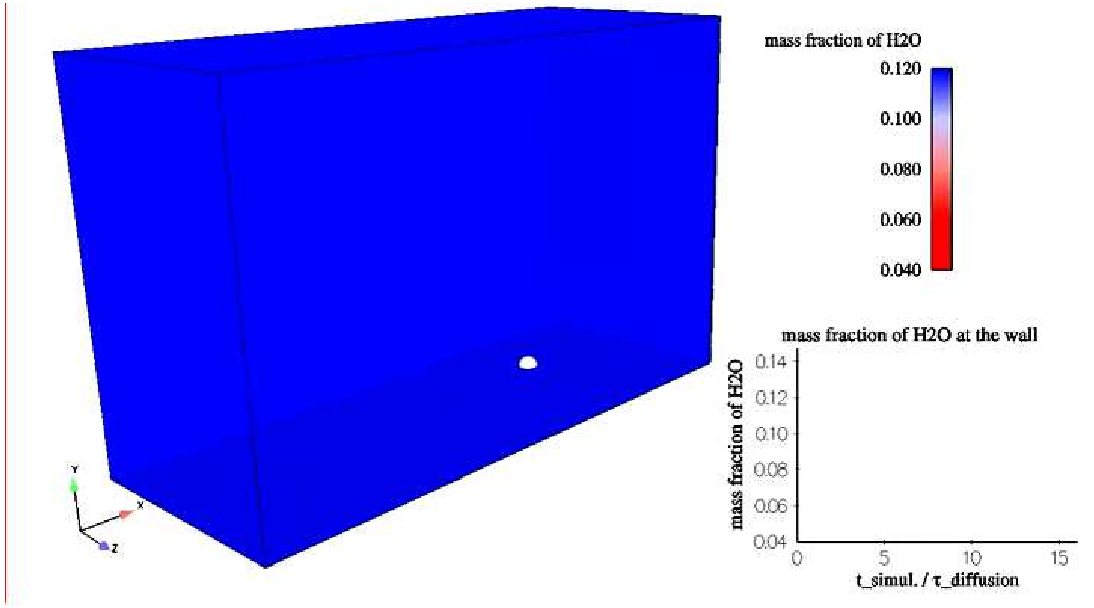
- Averages are not always enough (instabilities, growth rate, vortex shedding)

- Averages are even not always meaningful



MOTIVATION - 3

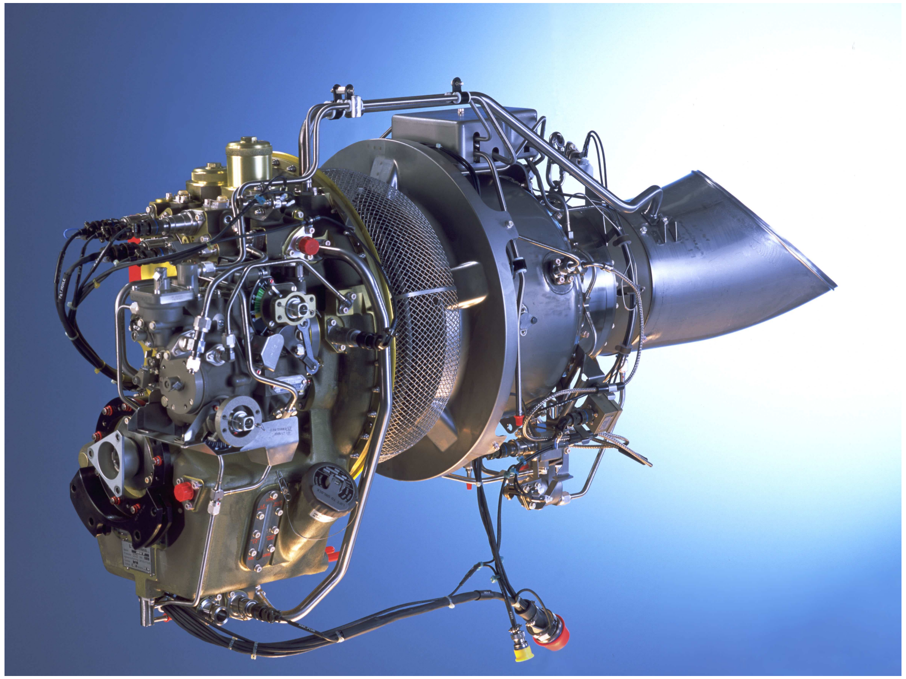
- Some phenomena are unsteady in nature.
  Ex: turbulence in a channel with ablation

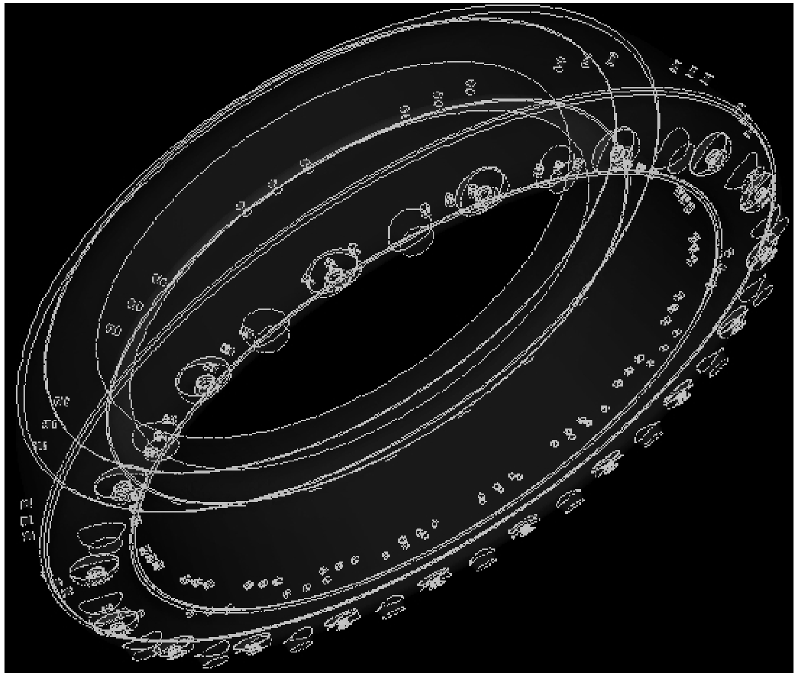


O. Cabrit – CERFACS & UM2

MOTIVATION - 4

- Some phenomena are unsteady in nature.
  Ex: ignition of an helicopter engine





Y. Sommerer & M. Boileau
CERFACS

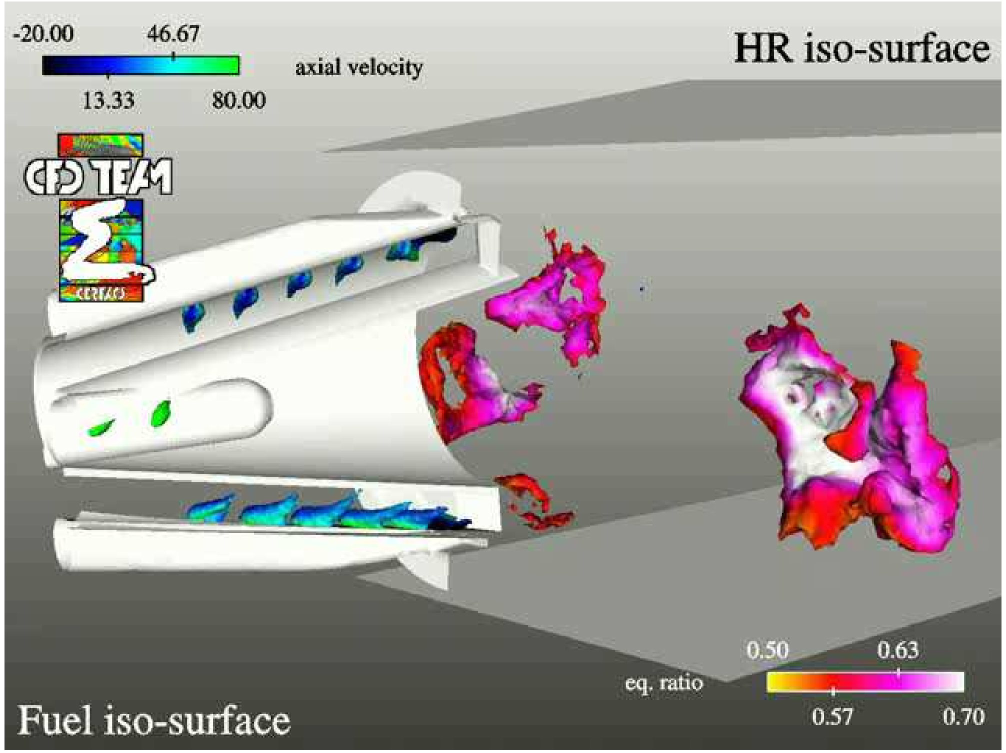
MOTIVATION - 5

- Some phenomena are unsteady in nature.
  Ex: thermoacoustic instability - Experiment

D. Durox, T. Schuller, S. Candel – EM2C

MOTIVATION - 6

- Some phenomena are unsteady in nature.
  Ex: thermoacoustic instability - CFD



P. Schmitt – CERFACS

PARALLEL COMPUTING

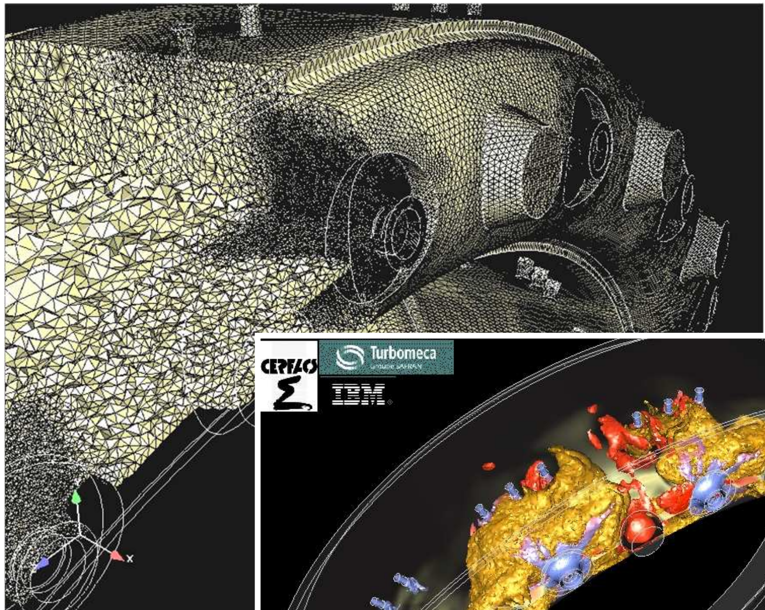
- www.top500.org – june 2007

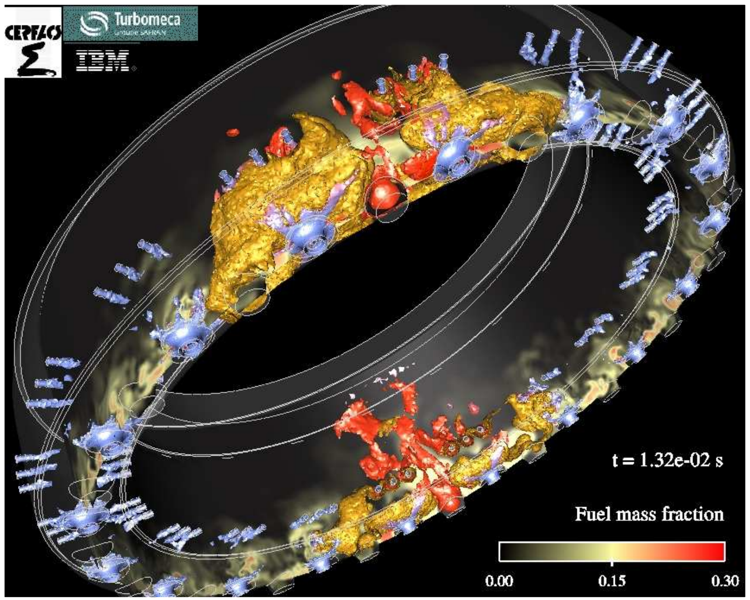
#	Site	Computer
1	DOE/NNSA/LLNL United States	BlueGene/L - eServer Blue Gene Solution IBM
2	Oak Ridge National Laboratory United States	Jaguar - Cray XT4/XT3 Cray Inc.
3	NNSA/Sandia National Laboratories United States	Red Storm - Sandia/ Cray Red Storm, Opteron 2.4 GHz dual core Cray Inc.
4	IBM Thomas J. Watson Research Center United States	BGW - eServer Blue Gene Solution IBM
5	Stony Brook/BNL, New York Center for Computional Sciences United States	New York Blue - eServer Blue Gene Solution IBM
6	DOE/NNSA/LLNL United States	ASC Purple - eServer pSeries p5 575 1.9 GHz IBM
7	Rensselaer Polytechnic Institute, Computional Center for Nanotechnology Innovations United States	eServer Blue Gene Solution IBM
8	NCSA United States	Abe - PowerEdge 1955, 2.33 GHz, Infiniband Dell
9	Barcelona Supercomputing Center Spain	MareNostrum - BladeCenter JS21 Cluster, PPC 970, 2.3 GHz, Myrinet IBM
10	Leibniz Rechenzentrum Germany	HLRB-II - Altix 4700 1.6 GHz SGI

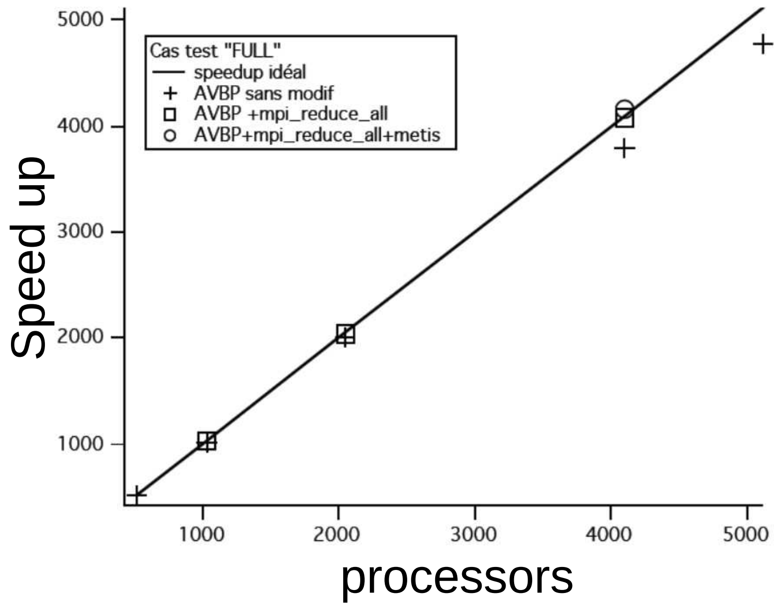
10 000 processors or more

PARALLEL COMPUTING

- Large scale unsteady computations require huge computing resources, an efficient codes …







SOME KEY INGREDIENTS

- **Flow physics**:
  - turbulence, combustion modeling, heat loss, radiative transfer, wall treatment, chemistry, two-phase flow, acoustics/flame coupling, mode interaction, …
- **Numerics**:
  - non-dissipative, low dispersion scheme, robustness, linear stability, non-linear stability, conservativity, high order, unstructured environment, parallel computing, error analysis, …
- **Boundary conditions**:
  - characteristic decomposition, turbulence injection, non-reflecting, pulsating conditions, complex impedance, …

BASIC EQUATIONS

reacting, multi-species gaseous mixture

$$\frac{\partial \rho_k}{\partial t} + \frac{\partial}{\partial x_j}(\rho_k\, u_j) = -\frac{\partial}{\partial x_j}[J_{j,k}] + \dot{\omega}_k.$$

$$\frac{\partial \rho\, u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho\, u_i\, u_j) = -\frac{\partial}{\partial x_j}[P\,\delta_{ij} - \tau_{ij}]$$

$$\frac{\partial \rho\, E}{\partial t} + \frac{\partial}{\partial x_j}(\rho\, E\, u_j) = -\frac{\partial}{\partial x_j}[u_i\,(P\,\delta_{ij} - \tau_{ij}) + q_j] + \dot{\omega}_T + Q_r.$$

$$P = \rho\, r\, T$$

$$r = \frac{R}{W} = \sum_{k=1}^{N} \frac{Y_k}{W_k}\mathcal{R} = \sum_{k=1}^{N} Y_k\, r_k$$

$$\rho h_s = \sum_{k=1}^{N} \rho_k h_{s,k} = \rho \sum_{k=1}^{N} Y_k h_{s,k}$$

$$h_{s,k}(T_i) = \int_{T_0=0K}^{T_i} C_{p,k} dT$$

$$J_{i,k} = -\rho\left(D_k \frac{W_k}{W}\frac{\partial X_k}{\partial x_i} - Y_k V_i^c\right)$$

$$q_i = \underbrace{-\lambda\frac{\partial T}{\partial x_i}}_{\text{Heat conduction}} \quad \underbrace{-\rho\sum_{k=1}^{N}\left(D_k \frac{W_k}{W}\frac{\partial X_k}{\partial x_i} - Y_k V_i^c\right) h_{s,k}}_{\text{Heat flux through species diffusion}}$$

SIMPLER BASIC EQUATIONS

- Navier-Stokes equations for a compressible fluid

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \qquad \frac{P}{\rho} = rT$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \qquad \tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\delta_{ij}\frac{\partial u_k}{\partial x_k}$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i E\right) = -\frac{\partial u_i\left(P\delta_{ij}\right)}{\partial x_j} + \frac{\partial u_i \tau_{ij}}{\partial x_j} - \frac{\partial q_j}{\partial x_j} \qquad q_i = -\lambda\frac{\partial T}{\partial x_i}$$

- Finite speed of propagation of pressure waves

SIMPLER BASIC EQUATIONS

- Navier-Stokes equations for an incompressible fluid

$$\frac{\partial u_i}{\partial x_i} = 0 \qquad \rho = \rho_0$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \qquad \tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- Infinite speed of propagation of pressure waves
- Contain turbulence

Turbulence

Turbulence

"I am an old man now, and when I die and go to Heaven there are two matters on which I hope enlightenment. One is quantum electro-dynamics and the other is turbulence.

About the former, I am really rather optimistic"

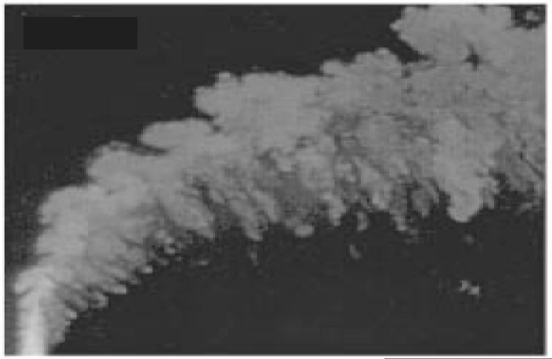
Sir Horace Lamb (1932)

From S. Goldstein, Ann. Rev. Fluid Mech, 1, 23 (1969)

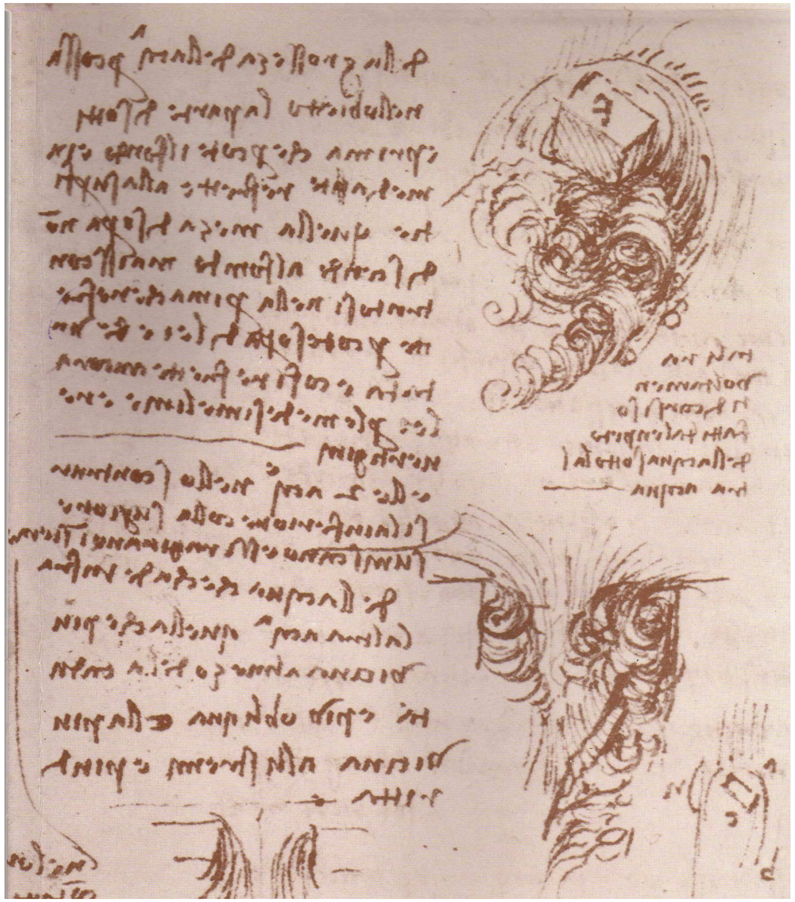
" What is turbulence ?
Turbulence is like pornography.
It is hard to define,
but if you see it, you recognize it immediately"

G. K. Vallis, 1999

TURBULENCE IS EVERYWHERE

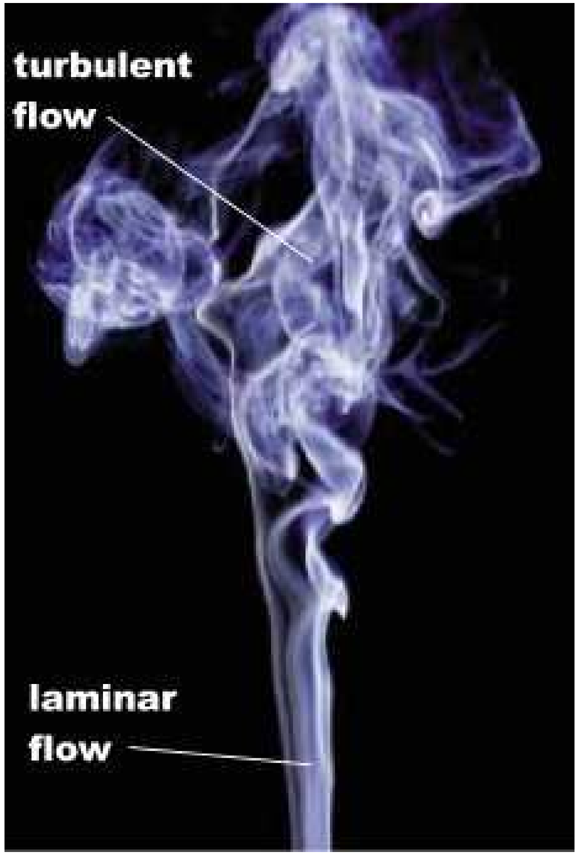


TURBULENCE



Leonardo da Vinci

TURBULENCE



The flow regime (laminar vs turbulent) depends on the Reynolds number :

Velocity — Length scale

$$\mathrm{Re} = \frac{Ud}{\nu}$$

ν — viscosity

laminar → turbulent

Re

TURBULENCE

- Turbulence is increasing mixing
  - Most often favorable (flames can stay in combustors)
  - Some drawbacks (drag, relaminarization techniques…)

TURBULENCE AND CHAOS

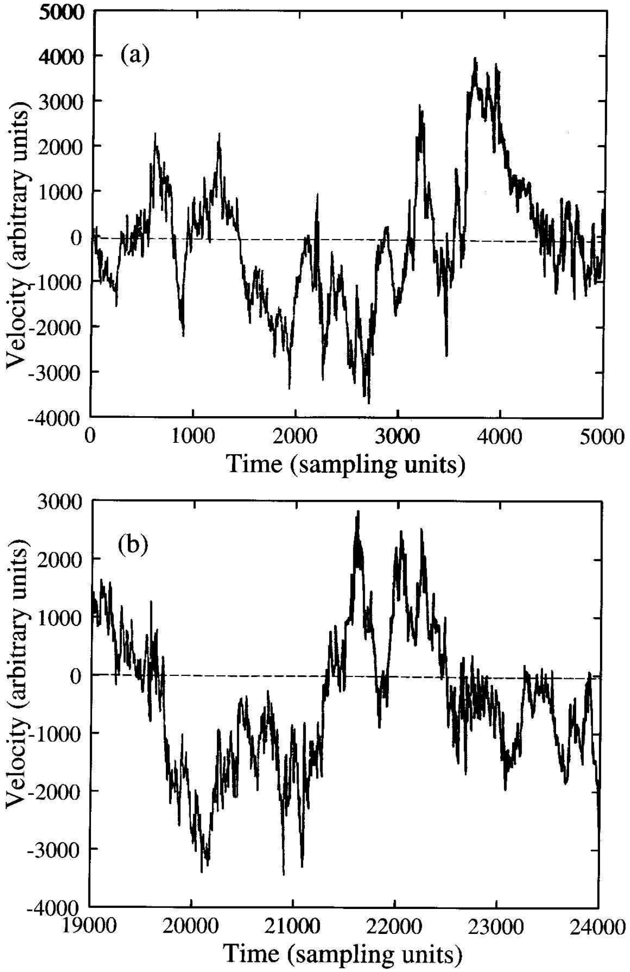


Fig. 3.1. One second of a signal recorded by a hot-wire (sampled at 5 kHz) in the S1 wind tunnel of ONERA (a); same signal, about four seconds later (b). Courtesy Y. Gagne and E. Hopfinger.

ONERA
WIND TUNNEL

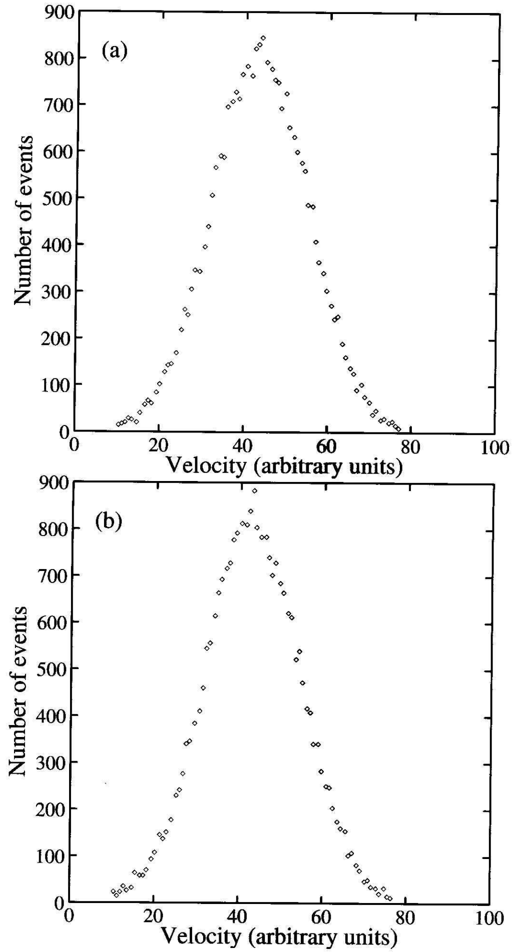
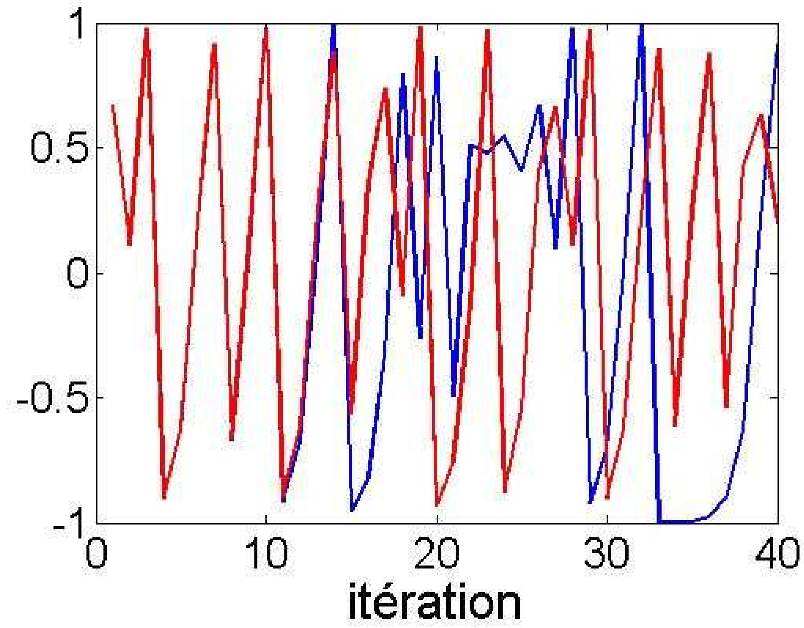


Fig. 3.3. Histogram for same signal as in Fig. 3.1(a), sampled 5000 times over a time-span of 150 seconds (a); same histogram, a few minutes later (b).

CHAOS OF THE POOR

$$v_{t+1} = 1 - 2v_t^2, \quad v_0 \in [-1,1]$$



$$v_0 = 0.6667 \qquad versus \qquad v_0 = 0.66667$$

TURBULENCE

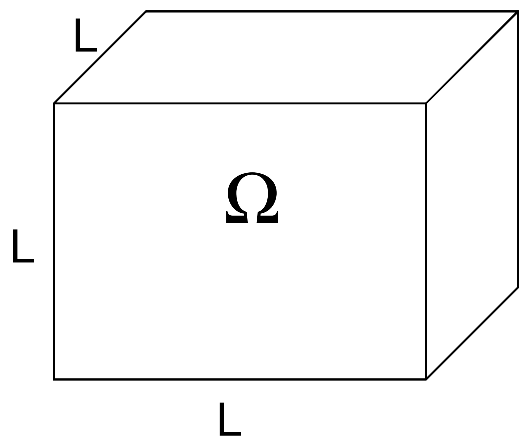
- The flow is very sensitive to the initial/boundary conditions. This leads to the impression of chaos, because the tiny details of the operating conditions are never known

- This sensitivity is related to the non-linear (convective) terms

- Need for an academic turbulent case

HOMOGENEOUS ISOTROPIC TURBULENCE

- No boundary
- L-periodic 3D domain
- $\phi(\mathbf{x}, t)$ being any physical quantity



$$\phi(\mathbf{x}, t) = \sum_{\mathbf{k}} \hat{\phi}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \mathbf{k} = \frac{2\pi}{L} Z^3$$

$$\hat{\phi}_k = \frac{1}{L^3} \iiint_{\Omega} \phi(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}} dx_1 dx_2 dx_3$$

BUDGETS IN HIT

- Spatial averaging $$\langle \phi \rangle (t) = \frac{1}{L^3} \iiint_{\Omega} \phi(\mathbf{x}) dx_1 dx_2 dx_3$$

- Momentum $$\frac{d\langle u_i \rangle}{dt} = 0$$

- Turbulent Kinetic Energy (TKE)

$$\frac{d\langle u_i^2 / 2 \rangle}{dt} = \underbrace{-\frac{\nu}{2}\left\langle \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)^2 \right\rangle}_{\varepsilon:\text{TKE dissipation rate}}$$

FLUX OF TKE

- For any K>0 and any $\phi(\mathbf{x},t)$

$$\phi^{<}(\mathbf{x},t)=\sum_{\mathbf{k}:|\mathbf{k}|<K}\hat{\phi}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \mathbf{k}=\frac{2\pi}{L}Z^{3}$$

- KE of scales larger than *2π/K*:

$$\frac{d\left\langle u_i^{<^2}/2\right\rangle}{dt}=-\varepsilon^{<}-\left\langle u_i^{<}u_j\frac{\partial u_i^{>}}{\partial x_j}\right\rangle$$

- Non linear terms are responsible for the energy transfer from the largest to the smallest scales

TURBULENCE: A SCENARIO

1. The largest scales of the flow are fed in energy (l_0)
   - Must be done at rate

$$\varepsilon \equiv \frac{u_0^3}{l_0}$$

2. The energy is transferred to smaller and smaller scales (l)
   - Must be done at rate

$$\varepsilon \equiv \frac{u^3}{l}$$

3. When scales become small enough (η), they become sensitive to the molecular viscosity and are eventually dissipated
   - Must occur when:

$$\frac{u_K \eta_K}{\nu} \equiv 1$$

SCALES IN TURBULENCE

- Kolmogorov scales (the smallest ones)

$$\eta_K \equiv \frac{\nu^{3/4}}{\varepsilon^{1/4}} \qquad\qquad u_K \equiv \nu^{1/4}\varepsilon^{1/4}$$

- Large-to-small scales ratio

$$\boxed{\frac{l_0}{\eta_K} \equiv R_0^{3/4}}$$

- Remark: in CFD, the number of grid points in each direction must follow the same scaling

TURBULENCE SPECTRUM

- Two-point correlation tensor:

$$R_{ij}(\mathbf{r}) = \left\langle u_i(\mathbf{x},t)u_j(\mathbf{x}+\mathbf{r},t)\right\rangle$$

- Velocity spectrum tensor

$$\phi_{ij}(\mathbf{k}) = \frac{1}{(2\pi)^3}\iiint_{R^3} R_{ij}(\mathbf{r})e^{-i\mathbf{k}\cdot\mathbf{r}}dr_1dr_2dr_3 \qquad R_{ij}(\mathbf{r}) = \iiint_{R^3} \phi_{ij}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}dk_1dk_2dk_3$$

- **Energy spectrum**: ***E(k)dk* is the kinetic energy contained in the scales whose wave number are between *k* and *k+dk***

$$E(k) = \frac{1}{2}\oint \phi_{ii}(\mathbf{k})dS(k)$$

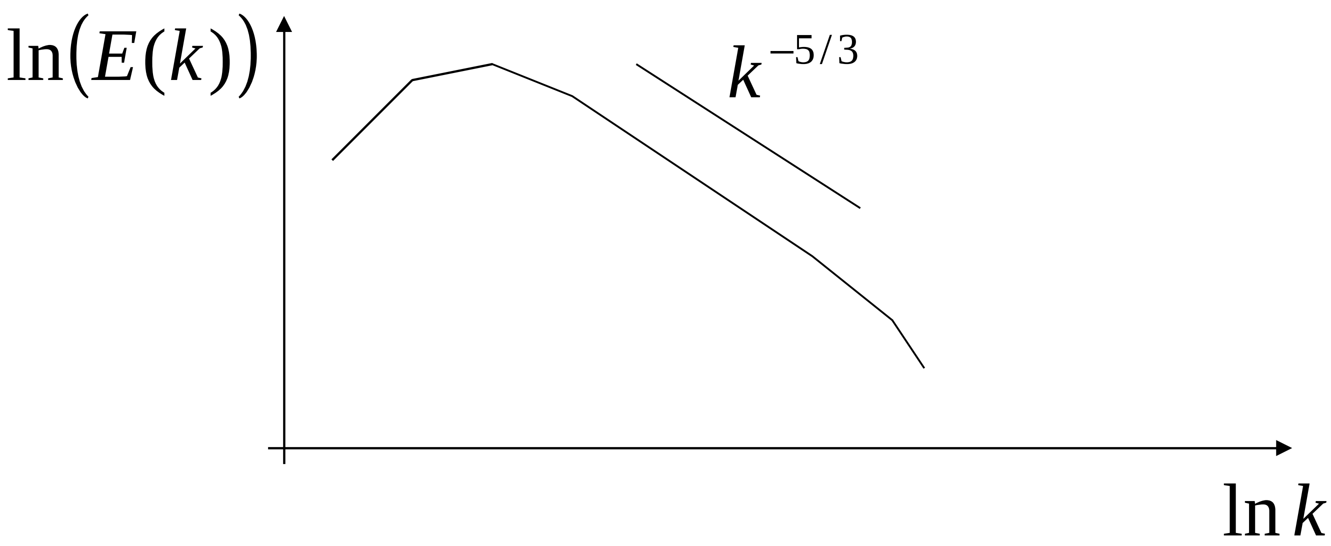
$$S(k)\text{: sphere of radius } k$$

$$\text{one shows that: } \int_0^\infty E(k)dk = \frac{1}{2}\left\langle u_i u_i\right\rangle$$

KOLMOGOROV ASSUMPTION

- After Kolmogorov (1941), there is an inertial zone ($l_0 << l << \eta$) where *E(k)* only depends on ε and *l* (viz. *k*).

It follows that: $$E(k) = C_K \varepsilon^{2/3} k^{-5/3}$$



TURBULENCE SPECTRUM

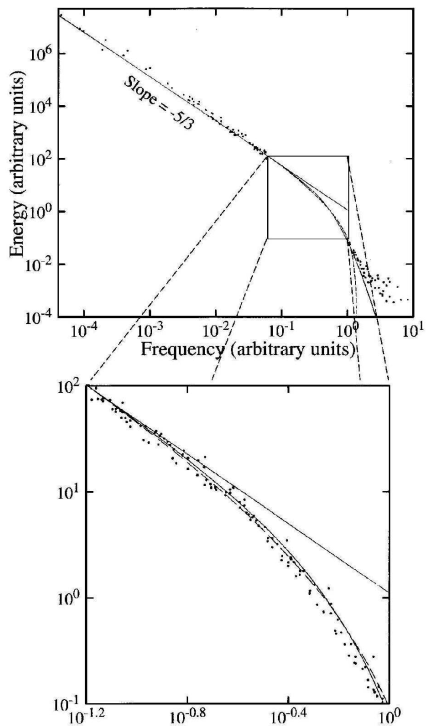


Fig. 5.5. log–log plot of the energy spectrum in the time domain and enlargement of the beginning of the dissipation range for tidal channel data (Grant, Stewart and Moilliet 1962).

CHANNEL

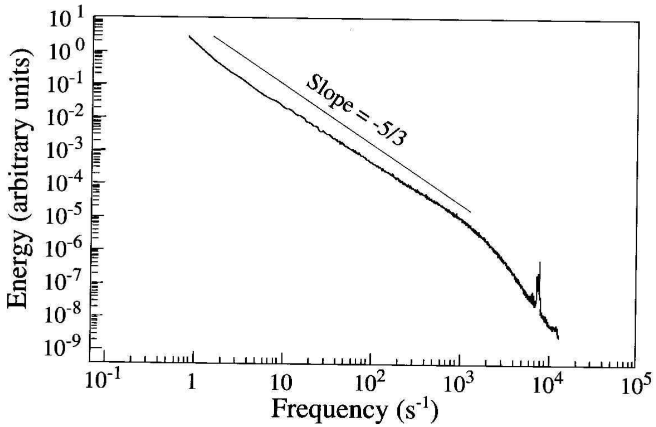


Fig. 5.4. Energy spectrum in the time domain for data from S1. Reynolds number $R_\lambda = 2720$. Courtesy Y. Gagne and M. Marchand.

ONERA WIND TUNNEL

JET

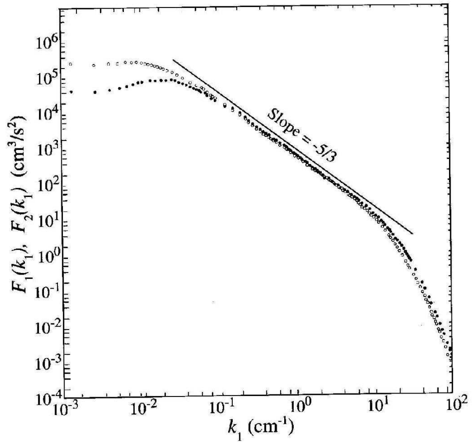


Fig. 5.7. log–log plot of the energy spectra of the streamwise component (white circles) and lateral component (black circles) of the velocity fluctuations in the time domain in a jet with $R_\lambda = 626$ (Champagne 1978).

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

Well supported by the experiments

TURBULENCE IN CFD

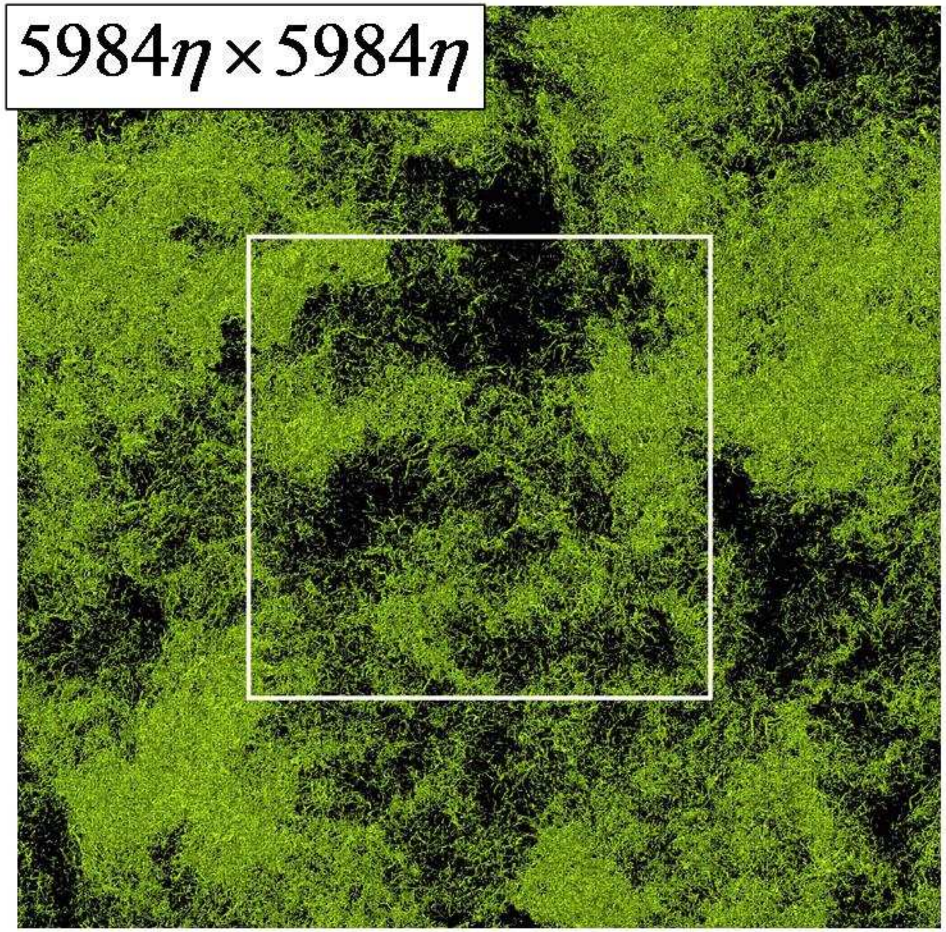
- Turbulence is contained in the Navier-Stokes equations

- So it is deterministic

- **BUT**: because the flow is so sensitive to the (unknown) details of IC and BC, only averages can be predicted, or used for comparison purposes
  ex: numerical/experimental comparisons

- “simply” resolve the Navier-Stokes equations to obtain turbulence: Direct Numerical Simulation

TURBULENCE IN CFD



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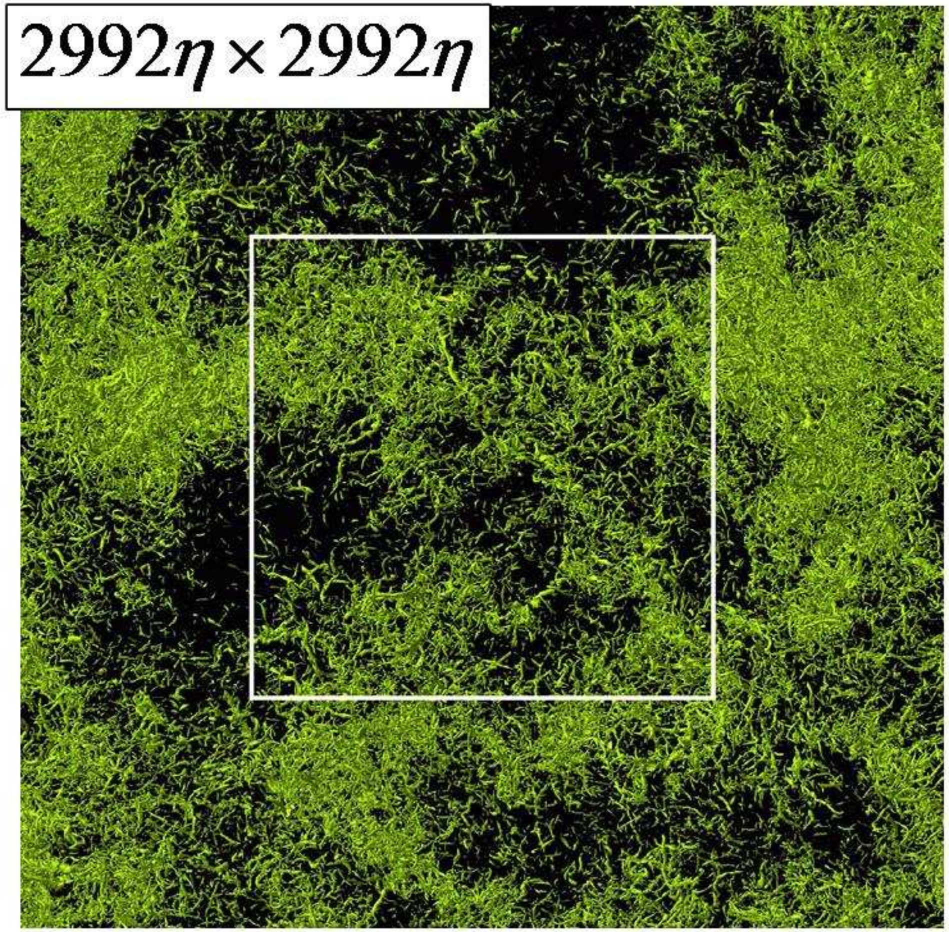
TURBULENCE IN CFD



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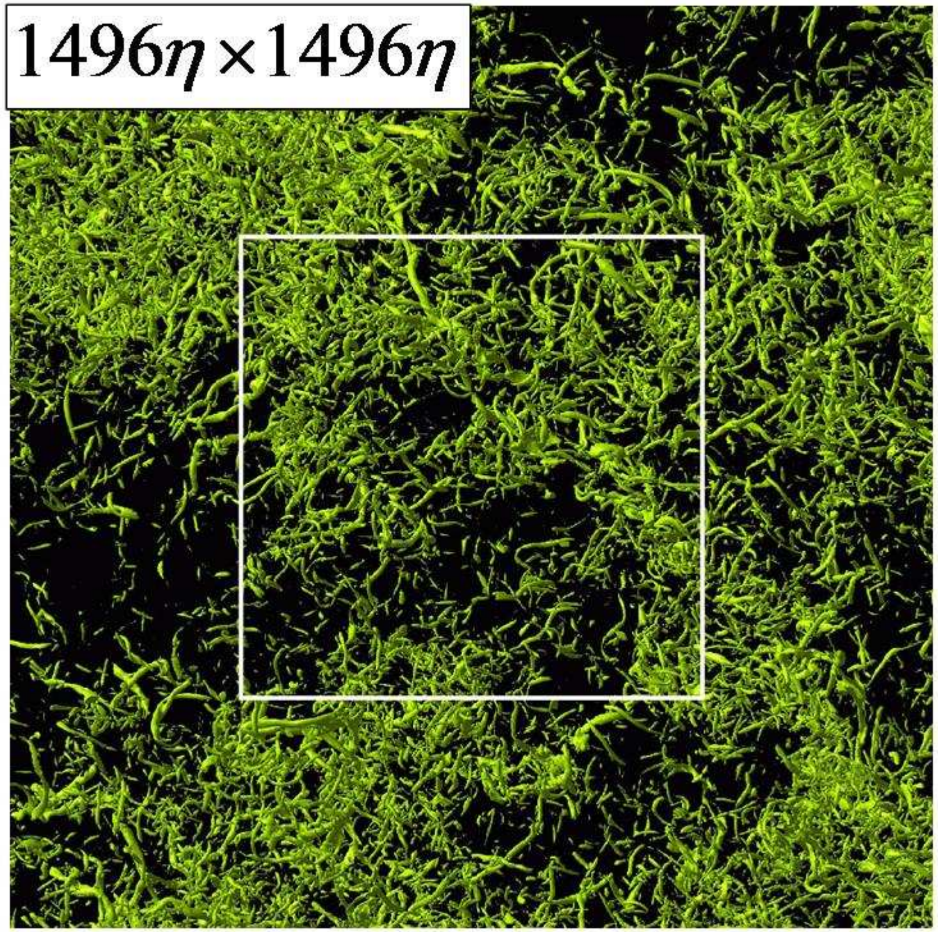
TURBULENCE IN CFD



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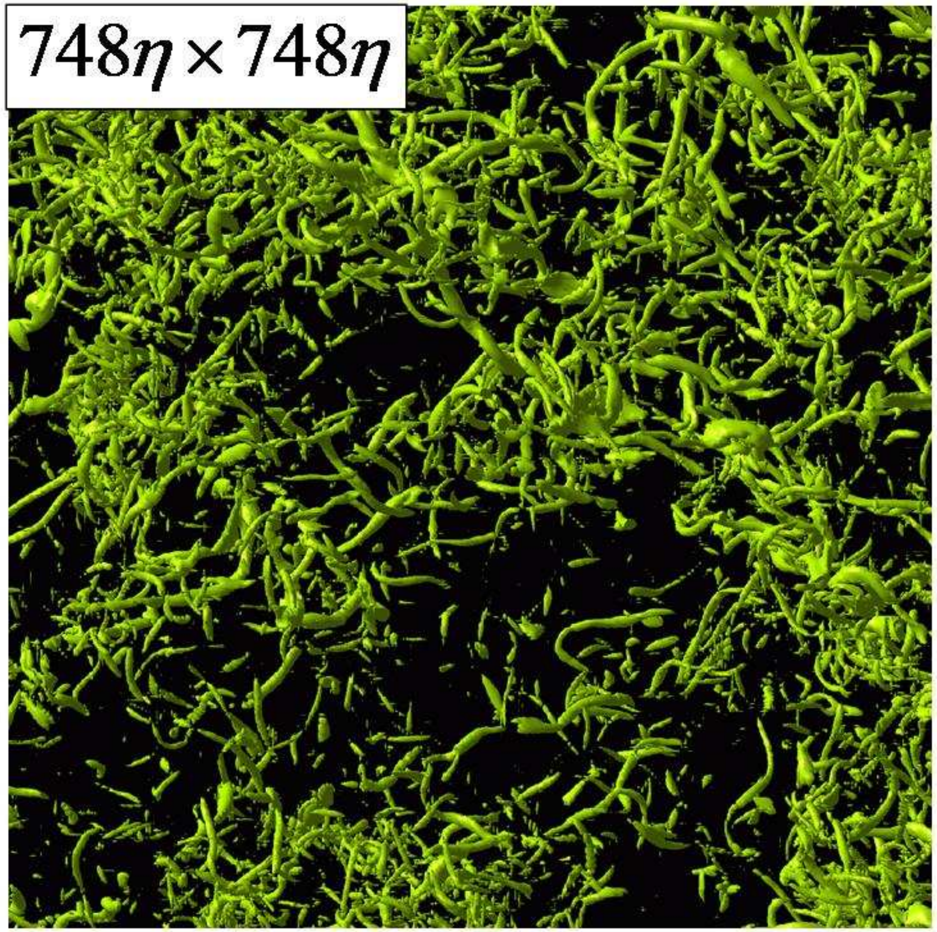
TURBULENCE IN CFD



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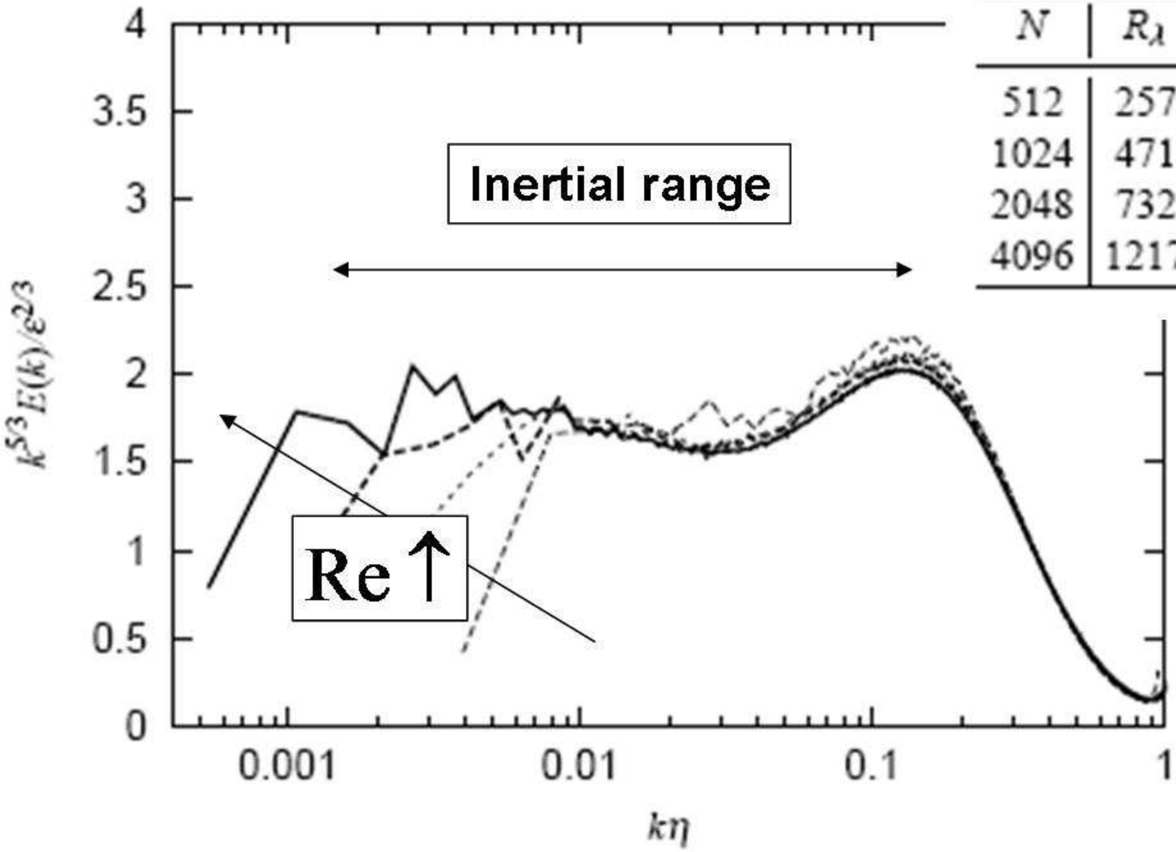
DNS OF ISOTROPIC TURBULENCE



N	R_λ	$\nu(\times 10^{-4})$	$\Delta t(\times 10^{-4})$	L	η
512	257	2.8	10.0	1.02	0.00395
1024	471	1.1	6.25	1.28	0.00210
2048	732	0.44	4.0	1.23	0.00105
4096	1217	0.173	2.5	1.21	0.00053

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DIRECT NUMERICAL SIMULATION OF TURBULENCE

- Solve the Navier-Stokes equations and represent all scales in space and time

- Compute the average, variance, of the unsteady solution

- The main limitation comes from the computer resources required:
  - the number of points required scales like $\left(R_0^{3/4}\right)^3 = R_0^{9/4}$
  - The CPU time scales like R_0^3

- In many practical applications, the Reynolds number is large, of order 10^6 or more

THE RANS APPROACH

- Ensemble average the (incompressible) Navier-Stokes equations

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0 \qquad \rho \frac{\partial \overline{u_i}}{\partial t} + \rho \frac{\partial \overline{u_i u_j}}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j}$$

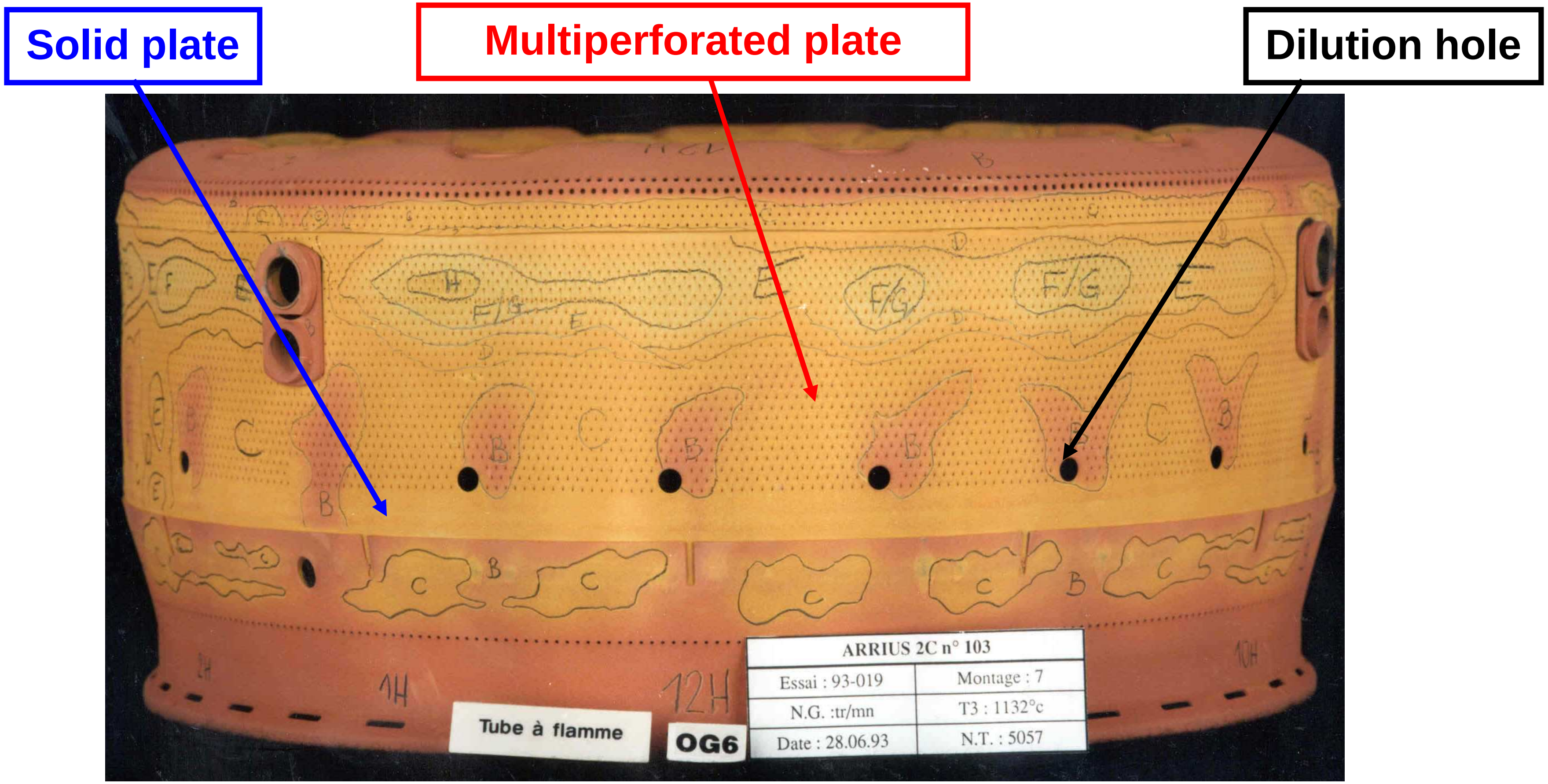
- Reynolds decomposition $u_i = \overline{u_i} + u_i'$

- Reynolds equations:

$$\boxed{\frac{\partial \overline{u_i}}{\partial x_i} = 0} \qquad \boxed{\rho \frac{\partial \overline{u_i}}{\partial t} + \rho \frac{\partial \overline{u_i}\,\overline{u_j}}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial \left(\overline{\tau_{ij}} - \rho \overline{u_i' u_j'}\right)}{\partial x_j}}$$

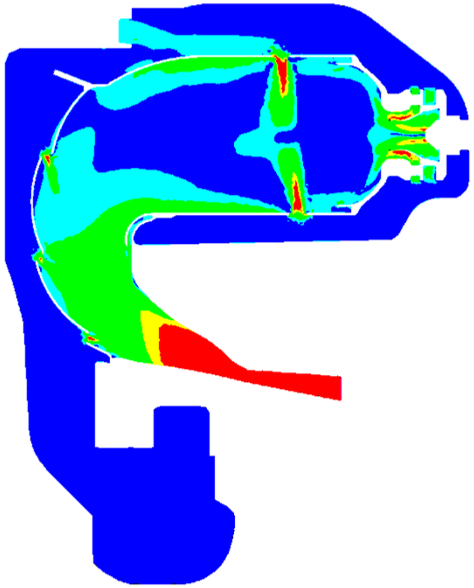
- A model for the Reynolds stress is required $-\rho \overline{u_i' u_j'}$

DNS vs RANS in a combustor



Modern combustion chamber - TURBOMECA

DNS vs RANS in a combustor



- **RANS**: used routinely during the design process.
- Approx. 10^6 nodes for the whole geometry

- **DNS**: used to know more about the flow physics in the multi-perforated plate region
- Approx. 10^6 nodes for only one perforation

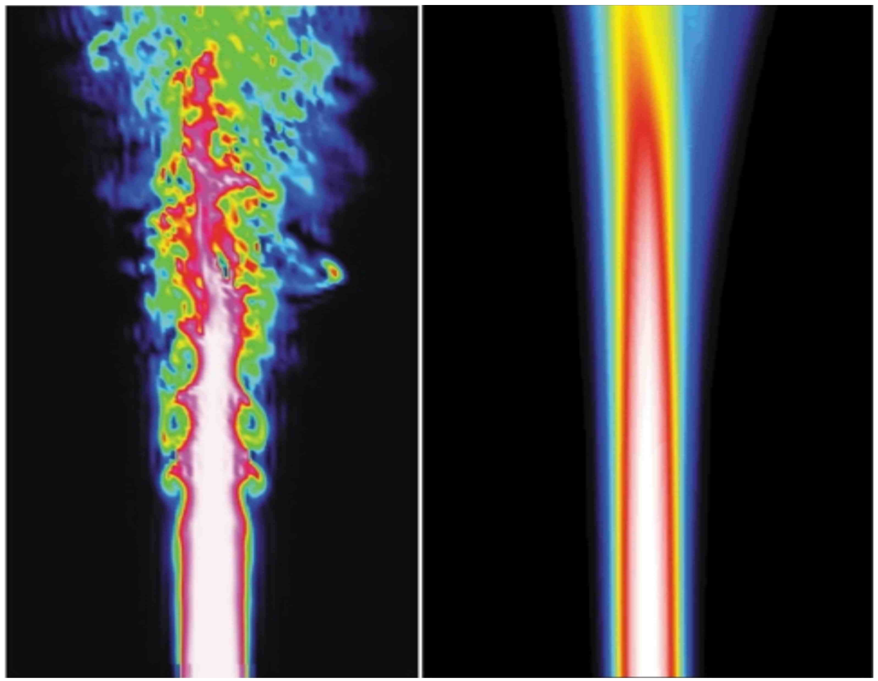
THE RANS APPROACH

- Intense scientific activity in the '70, '80 and '90 to derive the ultimate turbulence model.
  Ex: k-ε, RSM, k-ε-v^2, …

- No general model

- No flow dynamics

- Thanks to increasing available computer resources, unsteady calculations become affordable



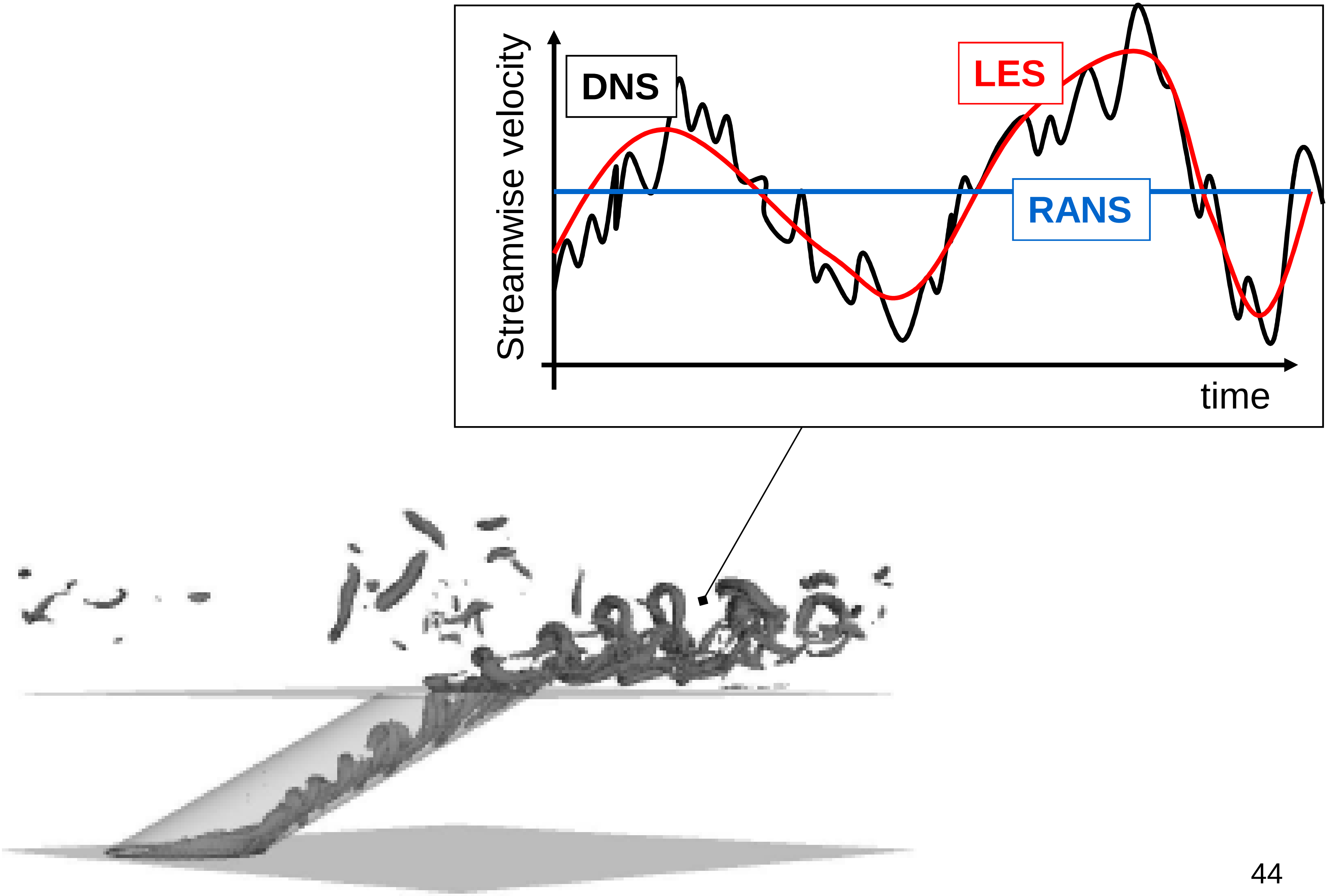
Jet of hot gas

RANS – LES - DNS

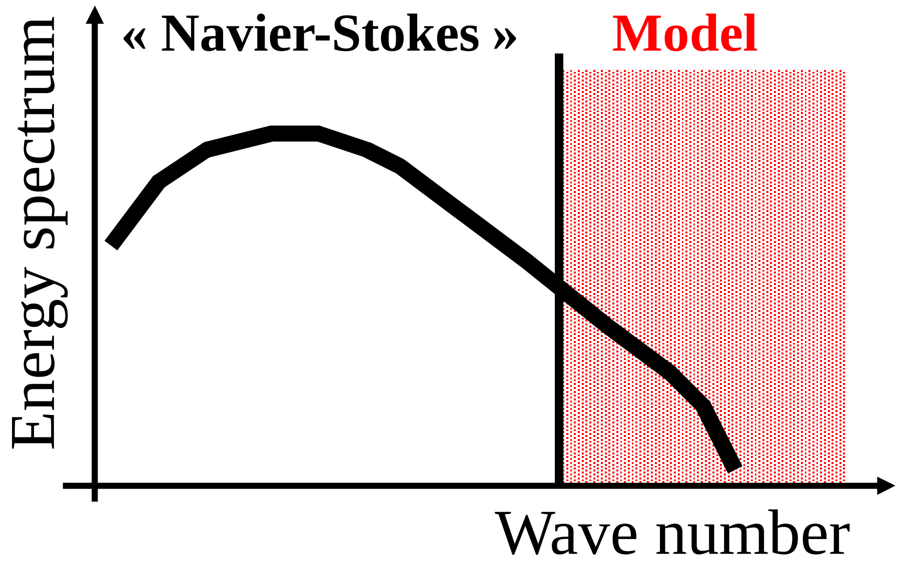
- **Reynolds-Averaged Navier-Stokes**:
  - Relies on a model to account for the turbulence effects
  - efficient but not predictive
- **Direct Numerical Simulation**:
  - The only model is Navier-Stokes
  - predictive but not tractable for practical applications
- **Large Eddy Simulation**:
  - Relies on a model for the smallest scales, more universal
  - Resolves the largest scales
  - Predictive and tractable

Large-Eddy Simulation

RANS – LES - DNS



Large Eddy Simulation



- Formally: replace the average operator by a spatial filtering to obtain the LES equations

$$\overline{\phi}(\mathbf{x},t)=\iiint_{R^3}\phi(\xi,t)G(\mathbf{x}-\xi)d^3\xi=G*\phi$$

LES equations

- Assumes small commutation errors

- Filter the incompressible equations to form $\overline{NS}$:

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0 \qquad \rho \frac{\partial \overline{u_i}}{\partial t} + \rho \frac{\partial \overline{u_i}\,\overline{u_j}}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial \left(\overline{\tau_{ij}} + \tau_{ij}^{sgs} \right)}{\partial x_j}$$

- Sub-grid scale stress tensor to be modeled

$$\tau_{ij}^{sgs} = \rho \overline{u_i}\,\overline{u_j} - \rho \overline{u_i u_j}$$

The Smagorinsky model

- From dimensional consideration, simply assume:

$$\tau_{ij}^{sgs} - \frac{1}{3}\tau_{kk}^{sgs}\delta_{ij} = 2\rho\nu_{sgs}\overline{S_{ij}}, \quad \text{with} \quad \overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial\overline{u_i}}{\partial x_j} + \frac{\partial\overline{u_j}}{\partial x_i}\right)$$

$$\boxed{\nu_{sgs} = (C_s\Delta)^2\sqrt{2\overline{S_{ij}}\,\overline{S_{ij}}}}$$

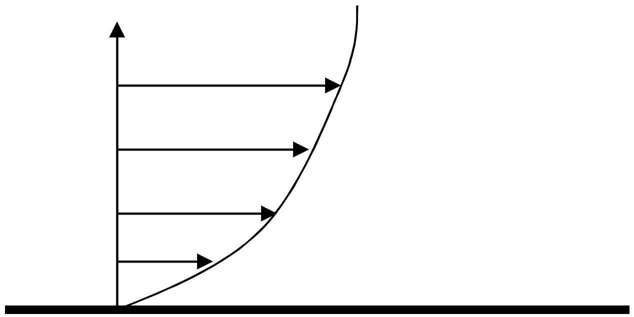
- The Smagorinsky constant is fixed so that the proper dissipation rate is produced, C_s =0.18

The Smagorinsky model

- The sgs dissipation is $\varepsilon_m = \tau_{ij}^{sgs}\overline{S_{ij}} \approx 2\rho\nu_{sgs}\overline{S_{ij}}\,\overline{S_{ij}}$ always positive

- Very simple to implement, no extra CPU time

- Any mean gradient induces sub-grid scale activity and dissipation, even in 2D !!



$$V = W = 0 \text{ but } \nu^{sgs} \neq 0$$

$$\text{because } U = U(y) \text{ and } S_{12} \neq 0$$

No laminar-to-turbulent transition possible

- Strong limitation due to its lack of universality.
  Eg.: in a channel flow, Cs=0.1 should be used

The Germano identity

- By performing $\overline{NS}$, the following sgs contribution appears

$$\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \left(\bar{\tau}_{ij} + \tau_{ij}^{sgs} \right)}{\partial x_j} \qquad \tau_{ij}^{sgs} = \rho \bar{u}_i \bar{u}_j - \rho \overline{u_i u_j}$$

- Let's apply another filter to these equations

$$\rho \frac{\partial \overleftrightarrow{\bar{u}_i}}{\partial t} + \rho \frac{\partial \overleftrightarrow{\bar{u}_i \bar{u}_j}}{\partial x_j} = -\frac{\partial \overleftrightarrow{\bar{P}}}{\partial x_i} + \frac{\partial \left(\overleftrightarrow{\bar{\tau}_{ij}} + \overleftrightarrow{\tau_{ij}^{sgs}} \right)}{\partial x_j} \qquad \overleftrightarrow{\tau_{ij}^{sgs}} = \rho \overleftrightarrow{\bar{u}_i \bar{u}_j} - \rho \overleftrightarrow{\overline{u_i u_j}}$$

A

- By performing $\overleftrightarrow{\overline{NS}}$, one obtains the following equations

$$\rho \frac{\partial \overleftrightarrow{\bar{u}_i}}{\partial t} + \rho \frac{\partial \overleftrightarrow{\bar{u}_i}\, \overleftrightarrow{\bar{u}_j}}{\partial x_j} = -\frac{\partial \overleftrightarrow{\bar{P}}}{\partial x_i} + \frac{\partial \left(\overleftrightarrow{\bar{\tau}_{ij}} + T_{ij}^{sgs} \right)}{\partial x_j} \qquad T_{ij}^{sgs} = \rho \overleftrightarrow{\bar{u}_i}\, \overleftrightarrow{\bar{u}_j} - \rho \overleftrightarrow{\overline{u_i u_j}}$$

B

- From **A** and **B** one obtains

$$T_{ij}^{sgs} = \overleftrightarrow{\tau_{ij}^{sgs}} - \rho \overleftrightarrow{\bar{u}_i \bar{u}_j} + \rho \overleftrightarrow{\bar{u}_i}\, \overleftrightarrow{\bar{u}_j}$$

The dynamic Smagorinsky model

- Assume the Smagorinsky model is applied twice

$$\tau_{ij}^{sgs} - \frac{1}{3}\tau_{kk}^{sgs}\delta_{ij} = 2\rho\left(C_s\overline{\Delta}\right)^2\sqrt{2\overline{S}_{ij}\,\overline{S}_{ij}}\;\overline{S}_{ij}$$

$$T_{ij}^{sgs} - \frac{1}{3}T_{kk}^{sgs}\delta_{ij} = 2\rho\left(C_s\overleftrightarrow{\overline{\Delta}}\right)^2\sqrt{2\overleftrightarrow{\overline{S}}_{ij}\,\overleftrightarrow{\overline{S}}_{ij}}\;\overleftrightarrow{\overline{S}}_{ij}$$

- Assume the same constant can be used and write the Germano identity

$$T_{ij}^{sgs} = \overleftrightarrow{\tau_{ij}^{sgs}} - \rho\overleftrightarrow{\overline{u}_i\,\overline{u}_j} + \rho\overleftrightarrow{\overline{u}}_i\,\overleftrightarrow{\overline{u}}_j$$

$$2\rho\left(C_s\overleftrightarrow{\overline{\Delta}}\right)^2\sqrt{2\overleftrightarrow{\overline{S}}_{ij}\,\overleftrightarrow{\overline{S}}_{ij}}\;\overleftrightarrow{\overline{S}}_{ij} + \frac{1}{3}T_{kk}^{sgs}\delta_{ij} = 2\rho\left(C_s\overline{\Delta}\right)^2\overleftrightarrow{\sqrt{2\overline{S}_{ij}\,\overline{S}_{ij}}\;\overline{S}_{ij}} + \frac{1}{3}\overleftrightarrow{\tau_{kk}^{sgs}}\delta_{ij} - \rho\overleftrightarrow{\overline{u}_i\,\overline{u}_j} + \rho\overleftrightarrow{\overline{u}}_i\,\overleftrightarrow{\overline{u}}_j$$

$$C_s^2 M_{ij} = N_{ij} + \frac{1}{3}\left(\overleftrightarrow{\tau_{kk}^{sgs}} - T_{kk}^{sgs}\right)\delta_{ij}$$

⇒ **C_s dynamically obtained from the solution itself**

The dynamic Smagorinsky model

- The model constant is obtained in the least mean square sense

$$C_s^2 = \frac{\left(N_{ij} + \frac{1}{3}\left(\overleftrightarrow{\tau_{kk}^{sgs}} - T_{kk}^{sgs}\right)\delta_{ij}\right)M_{ij}}{M_{ij}M_{ij}}$$

- No guaranty that $C_s^2 > 0$. Good news for the backscattering of energy; Bad news from a numerical point of view.

- In practice on takes $\overleftrightarrow{\overline{\Delta}} \approx 2\overline{\Delta}$

- Must be stabilized by some ad hoc procedure.
  E.g.: plan, Lagragian or local averaging

- Proper wall behavior

The dynamic Smagorinsky model

- The dynamic procedure is one of the reason for the development of LES in the last 15 years
- It allows to overcome the lack of universality of the Smagorinsky model
- The dynamic procedure can be (has been) applied to other models
  E.g.: dynamic determination of the sgs Prandtl number when computing the heat fluxes
- **BUT**:
  - it requires some ad hoc procedure to stabilize the computation
  - Defining a $\overleftrightarrow{\Delta} \approx 2\overline{\Delta}$ filter is not an easy task in complex geometries
- A static model with better properties than Smagorinsky ?

An improved static model

- From the eddy-viscosity assumption, modeling τ_{ij}^{sgs} means finding a proper expression for ν_{sgs}

- The Smagorinsky model reads

$$\nu_{sgs} = (C_s \Delta)^2 \sqrt{2 \overline{S}_{ij} \overline{S}_{ij}}$$

- More generally, from dimensional argument

$$\nu_{sgs} = C_m \, \Delta^2 \, \overline{OP}(\mathbf{x}, t), \quad \text{with} \quad \left[\overline{OP}(\mathbf{x}, t)\right] = T^{-1}$$

Dynamic procedure (C_m)

Natural choice (Δ^2)

Should depend on the filtered velocity. No necessarily equal to $\sqrt{2 \overline{S}_{ij} \overline{S}_{ij}}$ ($\overline{OP}(\mathbf{x}, t)$)

Choice of the frequency scale OP

- A good candidate appears to be based on the traceless symmetric part of the square of the velocity gradient tensor

$$\Sigma_{ij}^{d} = \frac{1}{2}\left(\bar{g}_{ij}^{2} + \bar{g}_{ji}^{2}\right) - \frac{1}{3}\bar{g}_{kk}^{2}\delta_{ij}$$

- Considering its second invariant

$$\Sigma_{ij}^{d}\Sigma_{ij}^{d} = \frac{1}{6}\left(S^{2}S^{2} + \Omega^{2}\Omega^{2}\right) + \frac{3}{2}S^{2}\Omega^{2} + 2IV_{S\Omega}$$

$$S^{2} = \bar{S}_{ij}\bar{S}_{ij} \qquad \Omega^{2} = \bar{\Omega}_{ij}\bar{\Omega}_{ij} \qquad IV_{S\Omega} = \bar{S}_{ik}\bar{S}_{kj}\bar{\Omega}_{jl}\bar{\Omega}_{li}$$

1. Involves both the strain and rotation rates
2. Exactly zero for any 2D field
3. Near solid walls, goes asymptotically to zero

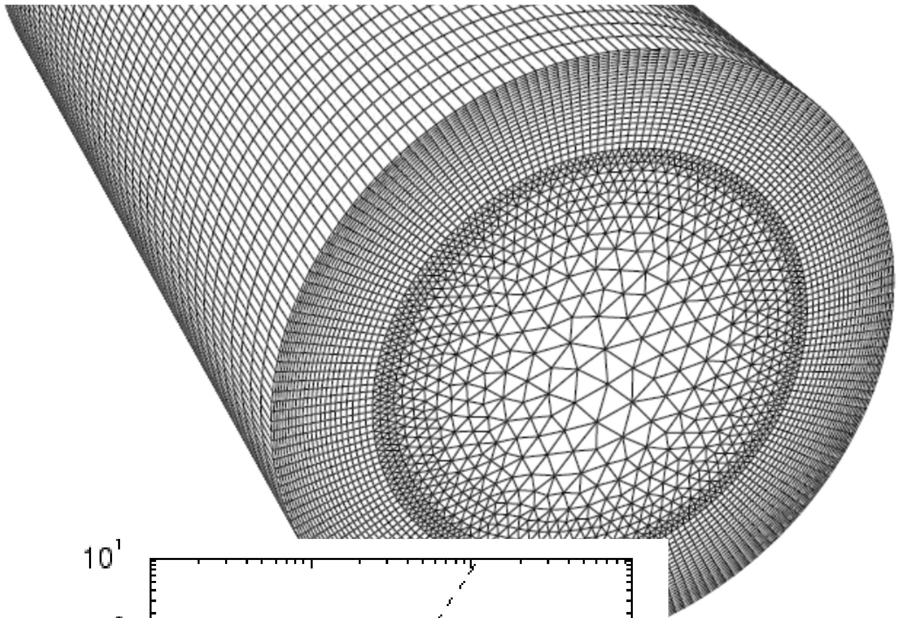
The Wall Adapting Local Eddy viscosity model

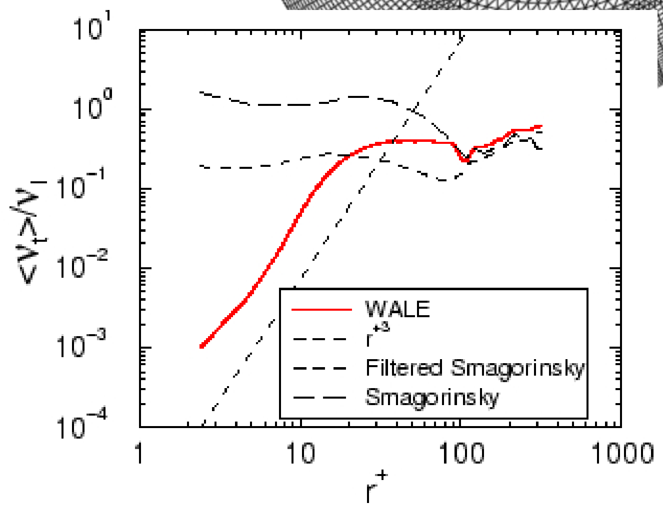
- The WALE model makes use of the previous invariant to define the sgs viscosity:

$$\nu_{sgs} = (C_m \Delta)^2 \frac{\left(\Sigma_{ij}^d \Sigma_{ij}^d\right)^{3/2}}{\left(\overline{S_{ij}}\,\overline{S_{ij}}\right)^{5/2} + \left(\Sigma_{ij}^d \Sigma_{ij}^d\right)^{5/4}}, \quad \text{with} \quad C_m = 0.5$$

1. Proper asymptotic behavior $\underbrace{\nu_{sgs} = O\left(y^3\right)}_{y \to 0}$
2. No extra filtering required
3. Simple implementation

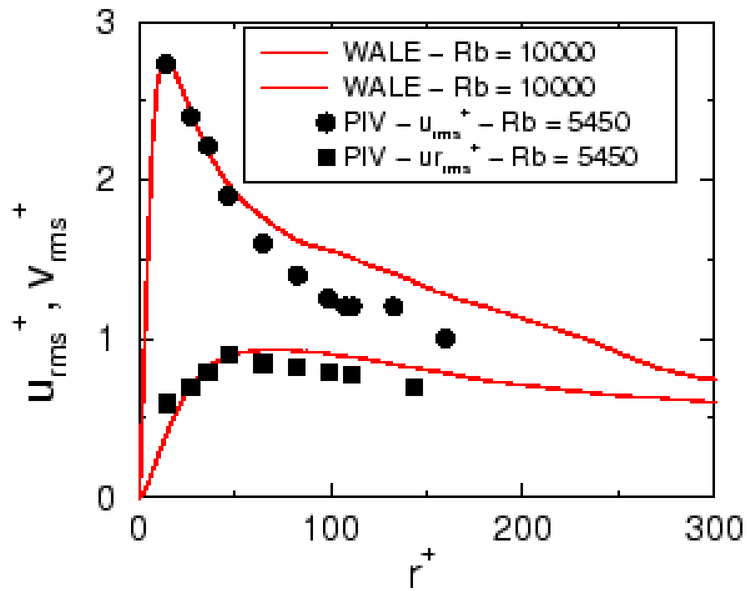
An academic case





Periodic cylindrical tube at bulk Reynolds number 10000

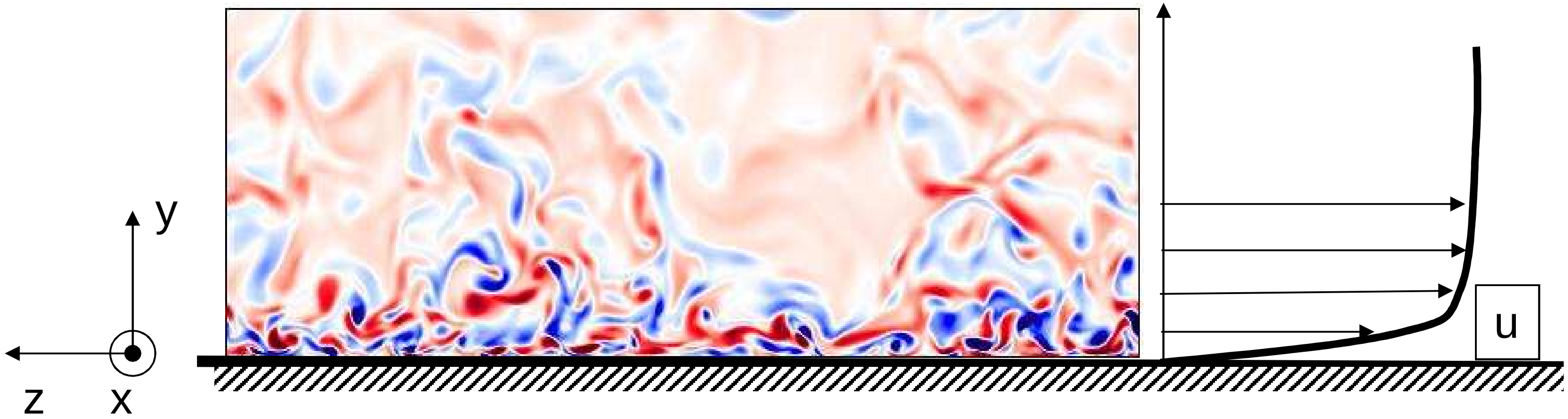
Simple geometry with complex mesh



About solid walls

- Close to solid walls, the largest scales are small …

Boundary layer along the x-direction: Vorticity ω_x



- steep velocity profile, $L_t \sim \kappa y$

- Resolution requirement: $\Delta y^+ = O(1)$, Δz^+ **and** $\Delta x^+ = O(10)$!!

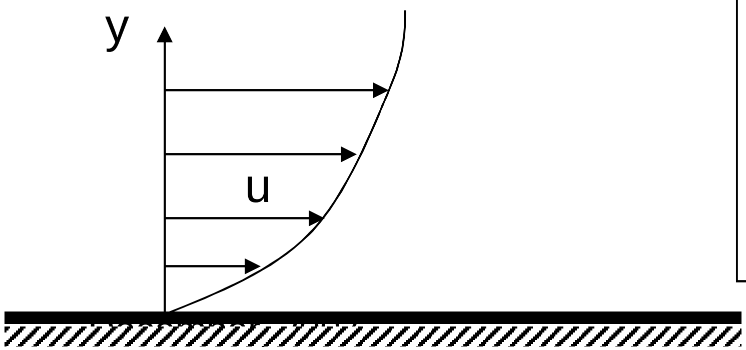
- Number of grid points: $O(R_\tau^2)$ for wall resolved LES

About solid walls

- In the near wall region, the total shear stress is constant. Thus the proper velocity and length scales are based on the wall shear stress τ_w:

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}} \qquad\qquad l = \frac{\nu}{u_\tau}$$

- In the case of attached boundary layers, there is an inertial zone where the following universal velocity law is followed



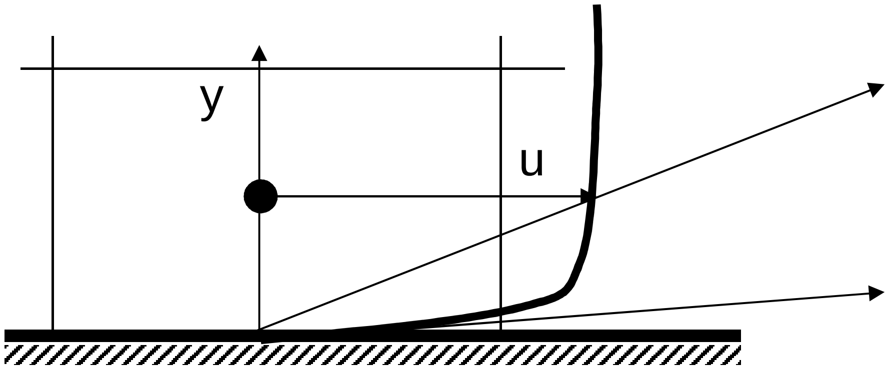
$$u^+ = \frac{1}{\kappa}\ln y^+ + C, \qquad u^+ = \frac{u}{u_\tau}, \qquad y^+ = \frac{y u_\tau}{\nu}$$

κ: Von Karman constant, $\kappa \approx 0.4$

C: "Universal constant", $C \approx 5.2$

Wall modeling

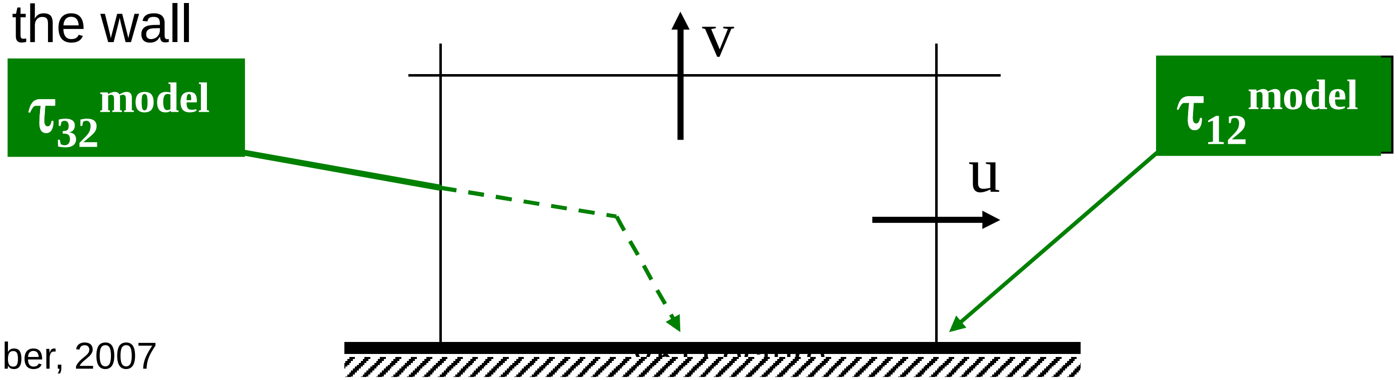
- A specific wall treatment is required to avoid huge mesh refinement or large errors,



Velocity gradient at wall assessed from a coarse grid

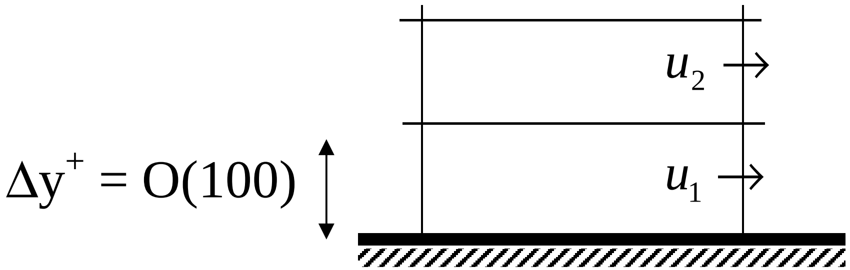
Exact velocity gradient at wall

- Use a coarse grid and the log law to impose the proper fluxes at the wall



Wall modeling in LES

- Coarse grid LES is not LES !!



$y_2 = 3\Delta y / 2$

$y_1 = \Delta y / 2$

Log. zone => $L = \kappa . y$

=> $L < \Delta y$!!
for j=1, 2

- Numerical errors are necessary large, even for the mean quantities

$$\left.\frac{du^+}{dy^+}\right|_{y^+=\Delta y^+} \approx \frac{u^+(3\Delta y^+/2) - u^+(\Delta y^+/2)}{\Delta y^+} \approx \frac{\ln 3}{\kappa \Delta y^+} \neq \frac{1}{\kappa \Delta y^+}$$

- No reliable model available yet

Numerical schemes for unsteady flows

Classical numerical methods

- Finite elements
- Finite volumes
- Finite differences

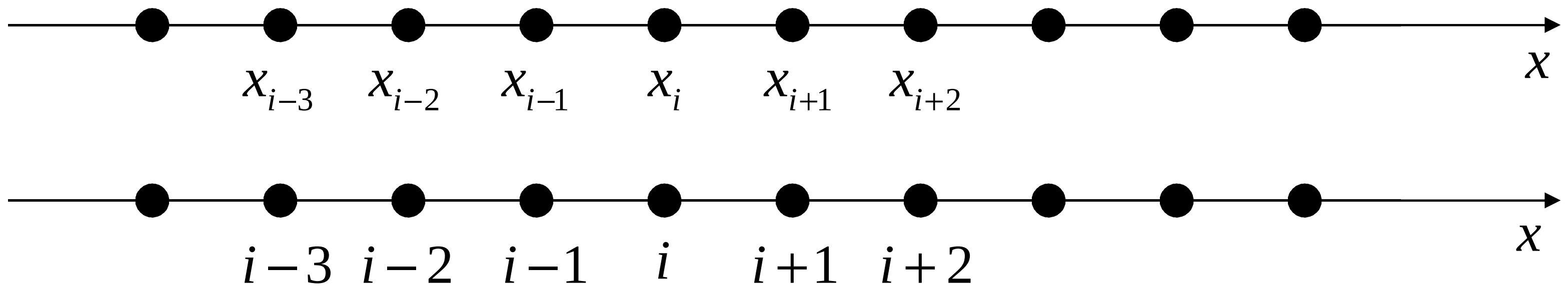
A few words about Finite Differences

- Finite differences are only adapted to Cartesian meshes
- The most intuitive approach
- In 1D, the three methods are equivalent
- Thus the FD are well suited to understand basic phenomena shared by the three methods

A few words about Finite Differences

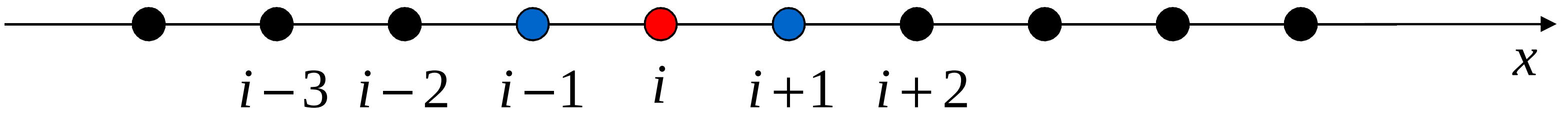
- Instead of seeking for $f(x)$, only the values of f at the nodes x_i are considered. Thus the unknowns are $f_i = f(x_i)$

- The basic idea is to replace each partial derivative in the PDE by expressions obtained from Taylor expansions written at node i



First spatial derivative

- Taylor expansion at node *i*:



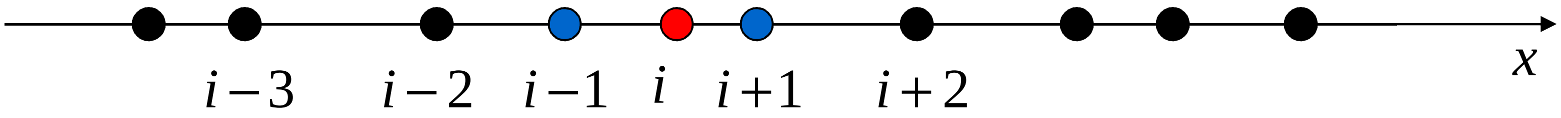
$$f_{i+1} = f_i + (x_{i+1} - x_i)\left.\frac{df}{dx}\right|_{x_i} + \frac{(x_{i+1} - x_i)^2}{2}\left.\frac{d^2 f}{dx^2}\right|_{x_i} + O\left((x_{i+1} - x_i)^3\right)$$

$$f_{i-1} = f_i + (x_{i-1} - x_i)\left.\frac{df}{dx}\right|_{x_i} + \frac{(x_{i-1} - x_i)^2}{2}\left.\frac{d^2 f}{dx^2}\right|_{x_i} + O\left((x_{i-1} - x_i)^3\right)$$

- Only derivatives at node *i* are involved

First spatial derivative

- Defining $\Delta_{i-1} = x_i - x_{i-1}$ and $\Delta_i = x_{i+1} - x_i$



$$\Delta_{i-1}{}^2 \times \qquad f_{i+1} = f_i + \Delta_i \left.\frac{df}{dx}\right|_{x_i} + \frac{\Delta_i{}^2}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_i} + O\left(\Delta_i^3\right)$$

$$\Delta_i{}^2 \times \qquad f_{i-1} = f_i - \Delta_{i-1} \left.\frac{df}{dx}\right|_{x_i} + \frac{\Delta_{i-1}{}^2}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_i} + O\left(\Delta_{i-1}{}^3\right)$$

$$\Delta_{i-1}^2 f_{i+1} - \Delta_i^2 f_{i-1} = f_i\left(\Delta_{i-1}^2 - \Delta_i^2\right) + \left(\Delta_{i-1}^2 \Delta_i + \Delta_i^2 \Delta_{i-1}\right)\left.\frac{df}{dx}\right|_{x_i} + O\left(\Delta_{i-1}^3 \Delta_i^3\right)$$

$$\boxed{\left.\frac{df}{dx}\right|_{x_i} = \frac{\Delta_{i-1}^2 f_{i+1} - f_i\left(\Delta_{i-1}^2 - \Delta_i^2\right) - \Delta_i^2 f_{i-1}}{\Delta_{i-1}\Delta_i\left(\Delta_{i-1} + \Delta_i\right)} + O\left(\Delta^2\right)}$$

Uniform mesh

- If the mesh is uniform then $\Delta_{i-1} = \Delta_i = \Delta x$ and one recovers the classical FD formula :

$$\left.\frac{df}{dx}\right|_{x_i} \approx D_1^0 f_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

- The truncation error is $O(\Delta x^2)$
- Second order centered scheme

Other classical FD formulae

$$\left.\frac{df}{dx}\right|_{x_i} \approx \frac{f_{i+1} - f_i}{\Delta x} + O(\Delta x)$$

Downwind 1st order

$$\left.\frac{df}{dx}\right|_{x_i} \approx \frac{f_i - f_{i-1}}{\Delta x} + O(\Delta x)$$

Upwind 1st order

$$\left.\frac{df}{dx}\right|_{x_i} \approx \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x} + O(\Delta x^2)$$

Downwind 2nd order

$$\left.\frac{df}{dx}\right|_{x_i} \approx \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2\Delta x} + O(\Delta x^2)$$

Upwind 2nd order

$$\left.\frac{df}{dx}\right|_{x_i} \approx \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x} + O(\Delta x^4)$$

Centered 4th order

$$\left.\frac{df}{dx}\right|_{x_i} \approx \frac{f_{i+3} - 9f_{i+2} + 45f_{i+1} - 45f_{i-1} + 9f_{i-2} - f_{i-3}}{60\Delta x} + O(\Delta x^6)$$

Centered 6th order

1D convection-diffusion equation

- Consider the convection-diffusion of a passive scalar *C(x,t)* in a 1D, infinite domain

$$\frac{\partial C}{\partial t}+U_0\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2},\quad C(x,0)=C_0(x),\quad \lim_{x\to\pm\infty}C(x,t)=0$$

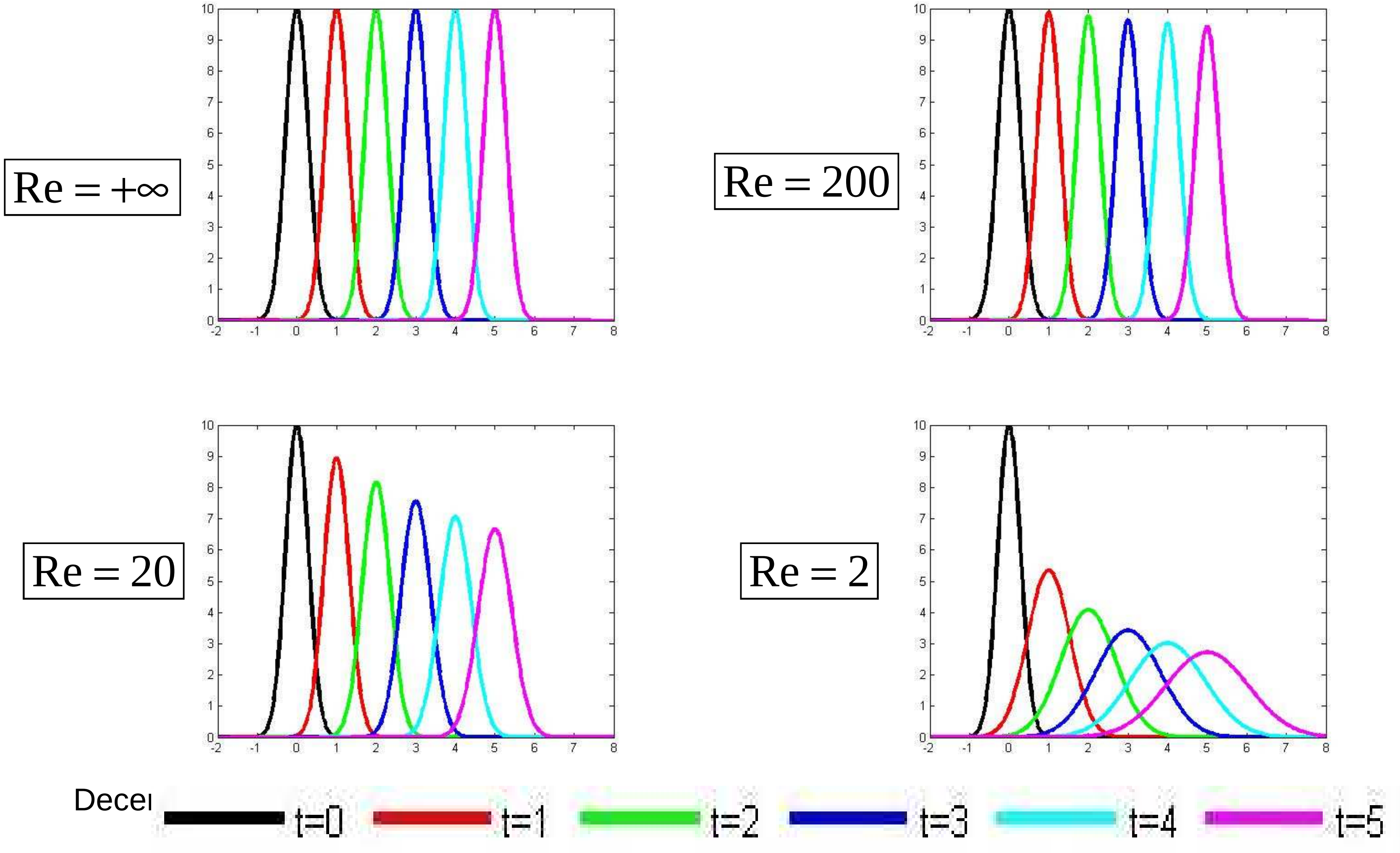
- Assuming a Gaussian initial condition one can derive the following analytical solution

$$\text{if}\quad C_0(x)=C_0\exp\left(-x^2/4a^2\right)\quad\text{then}$$

$$\boxed{C(x,t)=C_0\sqrt{\frac{a^2}{a^2+Dt}}\exp\left(-\frac{(x-U_0t)^2}{4\left(a^2+Dt\right)}\right)}$$

1D convection-diffusion equation

- Diffusion effect $\mathrm{Re} = \dfrac{U_0 \times a}{D}$



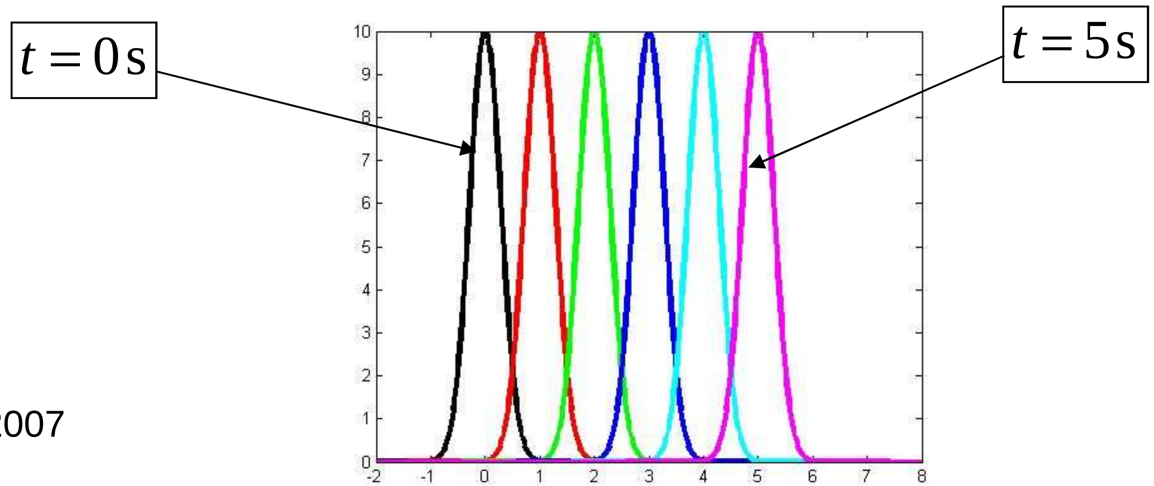
Comparing Schemes

- 1D convection equation (*D=0*)

$$\frac{\partial f}{\partial t} + U_0 \frac{\partial f}{\partial x} = 0, \quad -2\,\text{m} \le x \le 8\,\text{m}, \quad U_0 = 1\,\text{m/s}$$

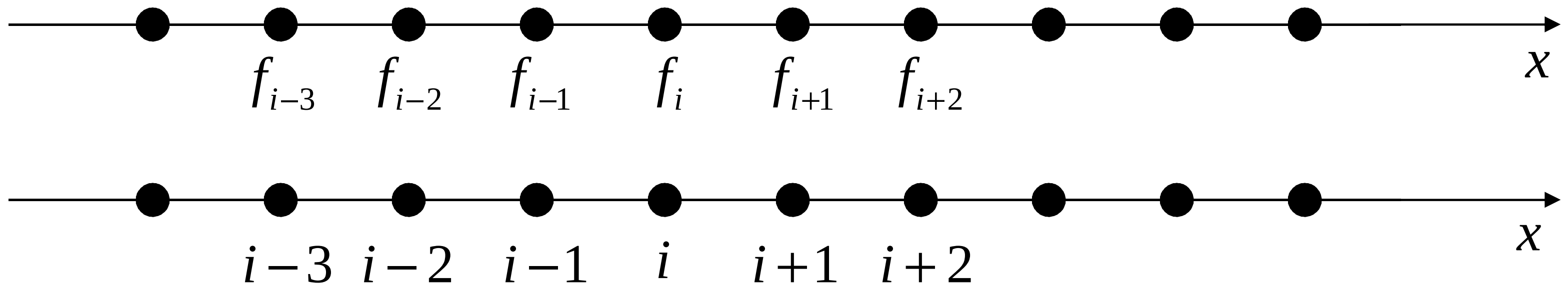
- Initial and boundary conditions:

$$f(x,0) = \exp\left(-x^2/4a^2\right), \quad a = 0.2\,\text{m} \qquad\qquad f(-2,t) = f(8,t) = 0$$



Numerical test

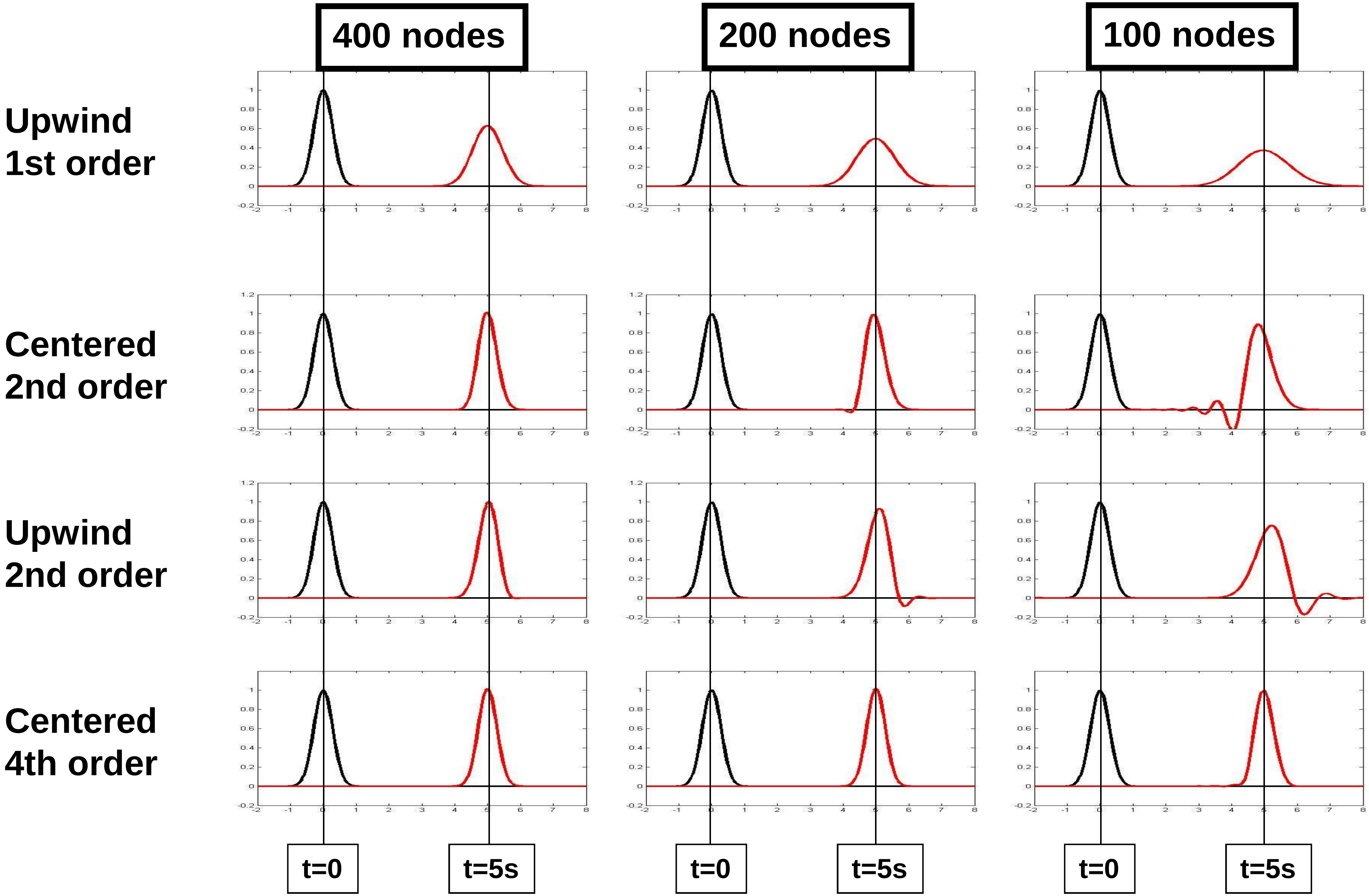
- Semi-discrete equation $\frac{df_i}{dt} + U_0 FD(f_i) = 0, \quad \forall i$



- No error associated with the time integration

- Compute the unknown f_i between t=0 and t=5s, using different FD formulae

Numerical test



Preliminary conclusions

- Upwind 1st order has a diffusive behavior …
- The 2nd order centered scheme is virtually exact with 400 nodes. The shape of the signal is strongly modified when only 100 nodes are used
- The 4th order centered scheme is virtually exact even with 100 nodes
- 4th better than the 2nd order; 2nd order better than 1st order
- The two 2nd order schemes behave differently regarding the speed of propagation, the shape of the signal, …
- A scheme cannot be characterized only by its order

Spectral analysis of spatial schemes

Spectral analysis

- Consider one single harmonic

$$f(x) = \mathrm{Re}[\exp(jkx)] \quad \Rightarrow \quad \frac{df}{dx} = \mathrm{Re}[jk\exp(jkx)]$$

- 2nd order centered scheme

$$f_i = \mathrm{Re}[\exp(jki\Delta x)], \quad \left.\frac{df}{dx}\right|_{x_i} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

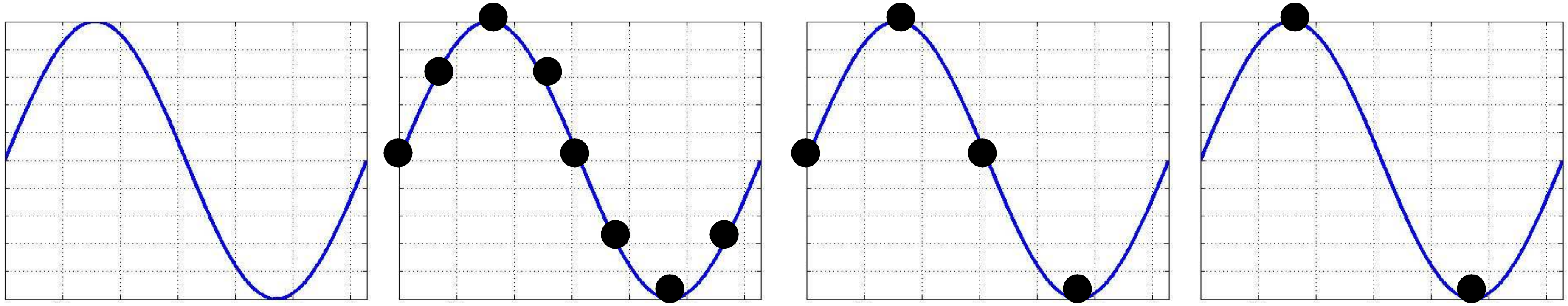
$$\left.\frac{df}{dx}\right|_{x_i} \approx \mathrm{Re}\left[jk\frac{\sin(k\Delta x)}{k\Delta x}\exp(jki\Delta x)\right]$$

- The "error" in the first derivative is $\boxed{\dfrac{\sin(k\Delta x)}{k\Delta x}}$

About the $k\Delta x$ *parameter*

- Consider one harmonic function of period *L* described with *N* points

- $\Delta x = L / N$, $k = 2\pi/L$ thus $k\Delta x = 2\pi / N$



$k\Delta x \to 0$ **(exact)**

$k\Delta x = \frac{\pi}{4}$

$k\Delta x = \frac{\pi}{2}$

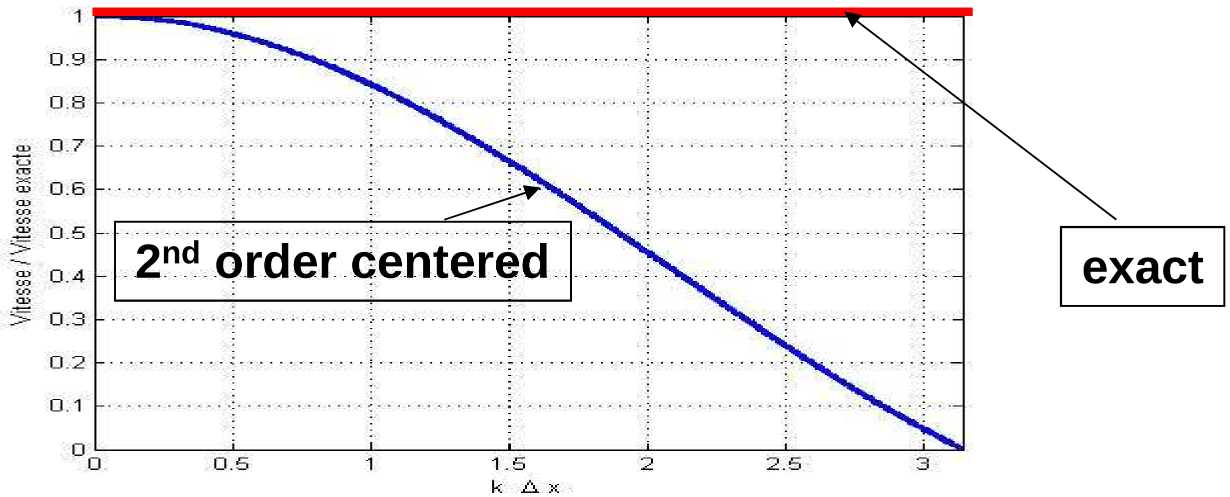
$k\Delta x = \pi$

Spectral analysis

- The effective equation that is solved is

$$\frac{\partial f}{\partial t} + U_0 \frac{\sin(k\Delta x)}{k\Delta x} \frac{\partial f}{\partial x} = 0$$

- Different wavelengths do not propagate at the same velocity

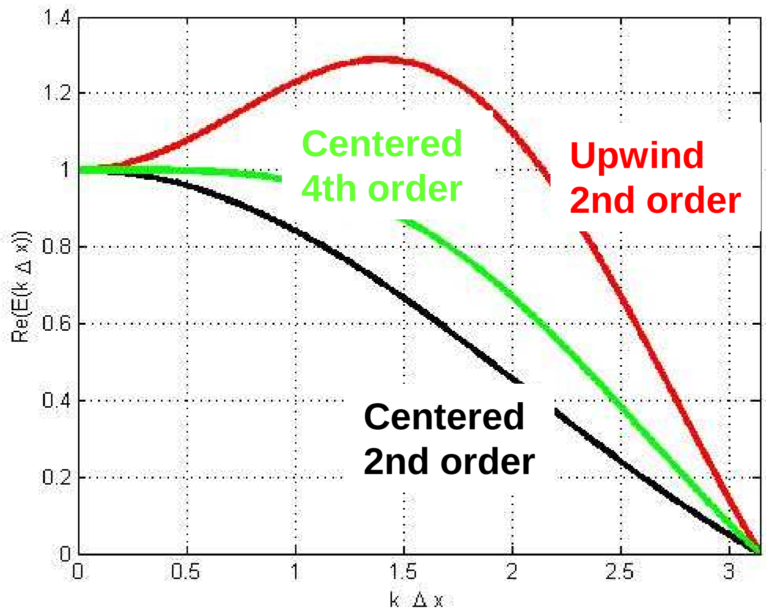


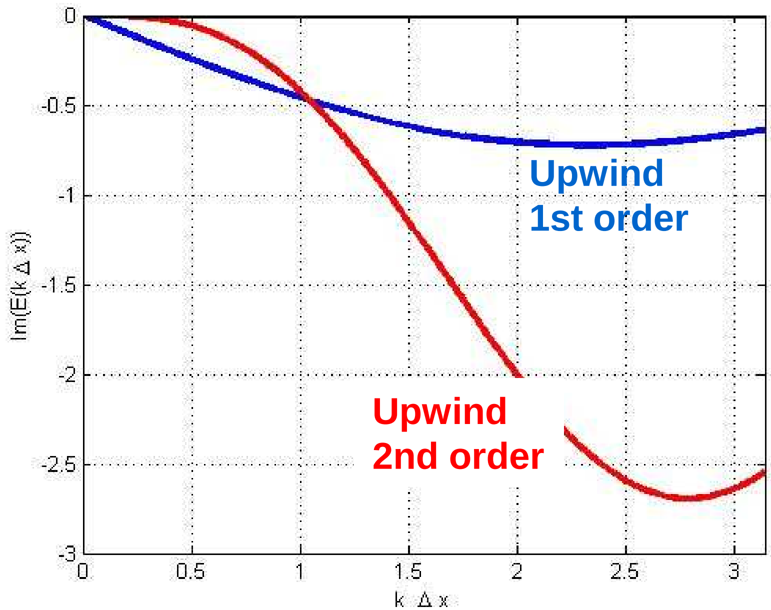
Spectral analysis

- Effective equation $\boxed{\dfrac{\partial f}{\partial t}+U_0E(k\Delta x)\dfrac{\partial f}{\partial x}=0} \quad \Rightarrow f=e^{jk(x-U_0E(k\Delta x)t)}$

SCHEME	$\mathrm{Re}\left[E(k\Delta x)\right]$	$\mathrm{Im}\left[E(k\Delta x)\right]$
2nd order centered	$\dfrac{\sin(k\Delta x)}{k\Delta x}$	0
1st order upwind	$\dfrac{\sin(k\Delta x)}{k\Delta x}$	$\dfrac{\cos(k\Delta x)-1}{k\Delta x}$
2nd order upwind	$\dfrac{\sin(k\Delta x)}{k\Delta x}\left(2-\cos(k\Delta x)\right)$	$\dfrac{-\cos(2k\Delta x)+4\cos(k\Delta x)-3}{k\Delta x}$
4th order centered	$\dfrac{\sin(k\Delta x)}{3k\Delta x}\left(4-\cos(k\Delta x)\right)$	0

Spectral analysis





When $k\Delta x$ tends to zero, $E(k\Delta x) = 1+O((k\Delta x)^n)$,
with n the scheme order

Dispersion

- The effective speed of propagation is equal to the exact one only in the liming case $k\Delta x \rightarrow 0$
- The actual speed of propagation of an harmonic perturbation depends on its wavelength
- Notably, the modes e^{jkx} and $e^{jk'x}, k \neq k'$ are not convected at the same speed
- What occurs when a multi-frequency function $f(x)$ propagates ?

Shape deformation

- Consider the function as a Fourier series

$$f(x) = \sum \hat{f}_k e^{jkx}$$

- The analytical solution at time *t* is

$$f(x - U_0 t) = \sum \hat{f}_k e^{jk(x - U_0 t)}$$

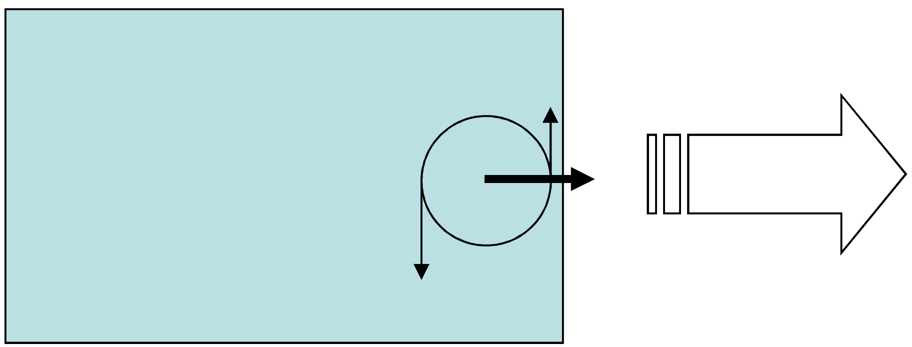
- Numerically, the mode e^{jkx} becomes $e^{jk(x - E(k\Delta x)U_0 t)}$

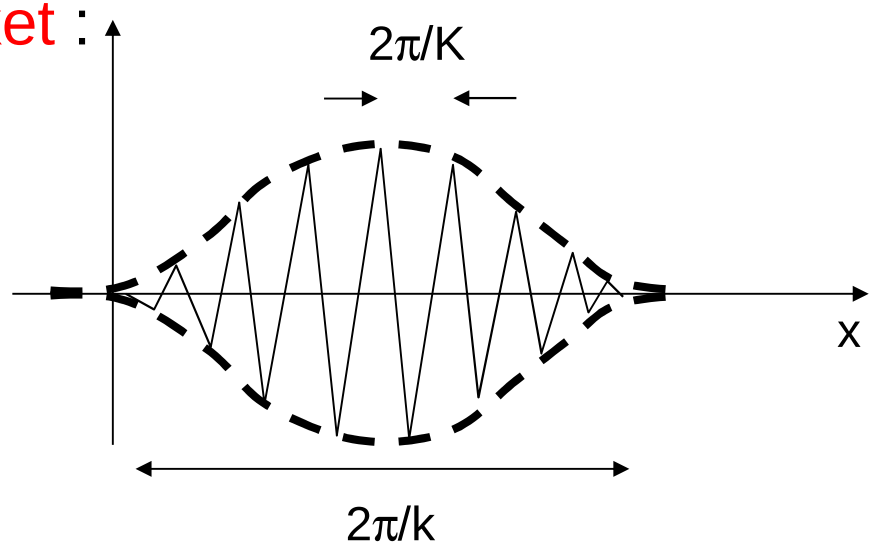
- Summing all contributions one obtains

$$f_{\mathrm{num}}(x - U_0 t) = \sum \underbrace{\hat{f}_k e^{jk(1 - E(k\Delta x))U_0 t}}_{\hat{g}_k \neq \hat{f}_k} e^{jk(x - U_0 t)} \neq f(x - U_0 t)$$

Another consequence of dispersion

- In practical computations, the solution may be polluted by high frequency numerical perturbations
- In practice, the numerical perturbations are not single harmonics
- Consider a simple wave packet :





$$f(x) = \mathrm{Re}\left[\exp(jkx + jKx)\right] \quad , \quad k << K$$

Group velocity

- Solve the 1D convection equation numerically, viz.

$$\boxed{\frac{\partial f}{\partial t} + U_0 E\big((k+K)\Delta x\big)\frac{\partial f}{\partial x} = 0} \quad \Rightarrow f = \exp\Big(j(k+K)\big(x - U_0 E\big((k+K)\Delta x\big)t\big)\Big)$$

- With $k \ll K$:

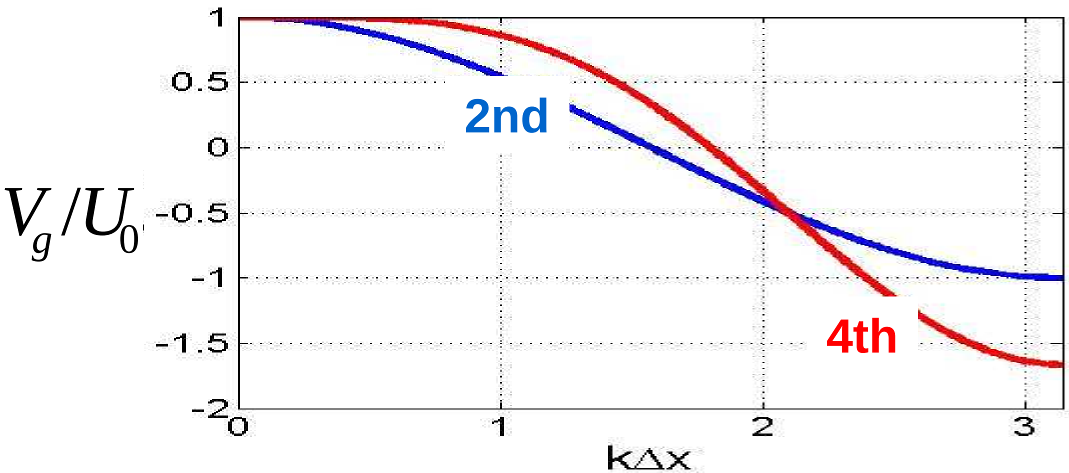
$$E\big((k+K)\Delta x\big) \approx E\big(K\Delta x\big) + k\frac{dE}{dK}(K\Delta x)$$

$$(k+K)\Big(x - U_0 E\big((k+K)\Delta x\big)t\Big) \approx K\Big(x - U_0 E\big(K\Delta x\big)t\Big) + k\left(\underbrace{x - U_0 E\big(K\Delta x\big)t - KU_0\frac{dE}{dK}\big(K\Delta x\big)t}_{-U_0\frac{dKE}{dK}(K\Delta x)t}\right)$$

Group velocity

Group velocity

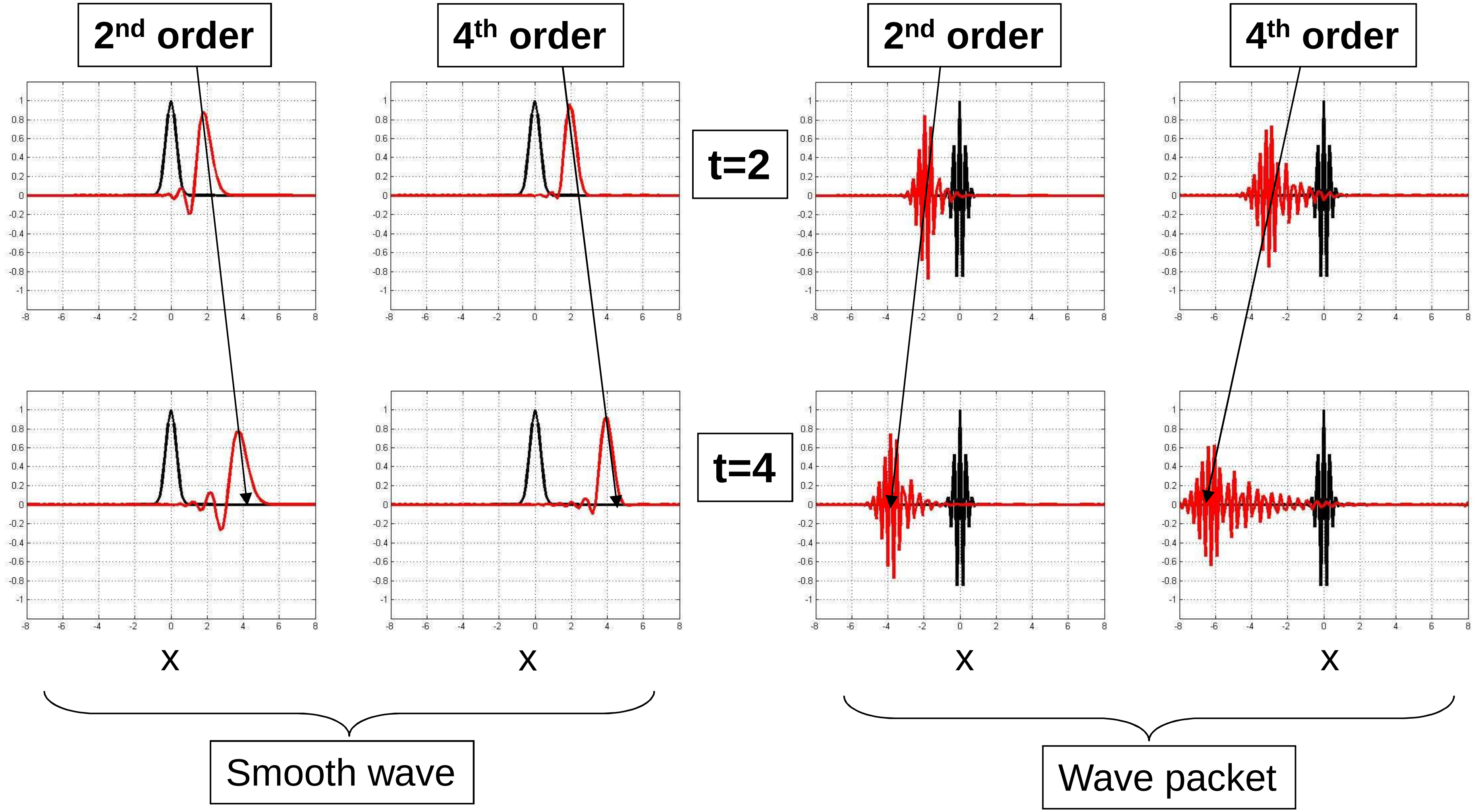
SCHEME	$E(K\Delta x)$	$V_g = U_0 \dfrac{dKE}{dK}$
2nd order centered	$\dfrac{\sin(K\Delta x)}{K\Delta x}$	$U_0 \cos(K\Delta x)$
4th order centered	$\dfrac{\sin(K\Delta x)}{3K\Delta x}\left(4-\cos(K\Delta x)\right)$	$\dfrac{U_0}{3}\left(4\cos(K\Delta x)-\cos(2K\Delta x)\right)$



Wiggles can propagate upstream !

The more accurate the scheme, the largest the group velocity

Numerical test $\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} = 0$



Stabilizing computations

Non linear stability

- Ensuring the linear stability is sometimes not enough, especially when performing LES or DNS of turbulent flows

- Recall the budget of TKE in isotropic turbulence

$$\frac{d\langle u_i^2/2\rangle}{dt} = \underbrace{-\frac{\nu}{2}\left\langle\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)^2\right\rangle}_{\varepsilon:\text{TKE dissipation rate}}$$

- So in the inviscid limit, in absence of external forcing, the TKE should be conserved
- Most of the numerical schemes do not meet this property

A 1D model example

- Consider the 1D Burgers equation in a L-periodic domain

$$\frac{\partial u}{\partial t}+\frac{\partial u^2}{\partial x}=0$$

- Multiply by *u*, integrate over space:

$$\frac{d\left\langle u^2/2\right\rangle}{dt}+\underbrace{\int_{x=0}^{L} u\frac{\partial u^2}{\partial x}dx}_{I}=0 \qquad I=\int_{x=0}^{L} u\frac{\partial u^2}{\partial x}dx=2\int_{x=0}^{L} u^2\frac{\partial u}{\partial x}dx=\frac{2}{3}\left[u^3\right]_{x=0}^{L}=0$$

$$\boxed{\frac{d\left\langle u^2/2\right\rangle}{dt}=0, \quad \left\langle\phi\right\rangle=\int_{x=0}^{L}\phi dx}$$

Numerical test

- Solve the Burgers equation in a 1D periodic domain with random initialization

- Use a small time step to minimize the error due to time integration (RK4)

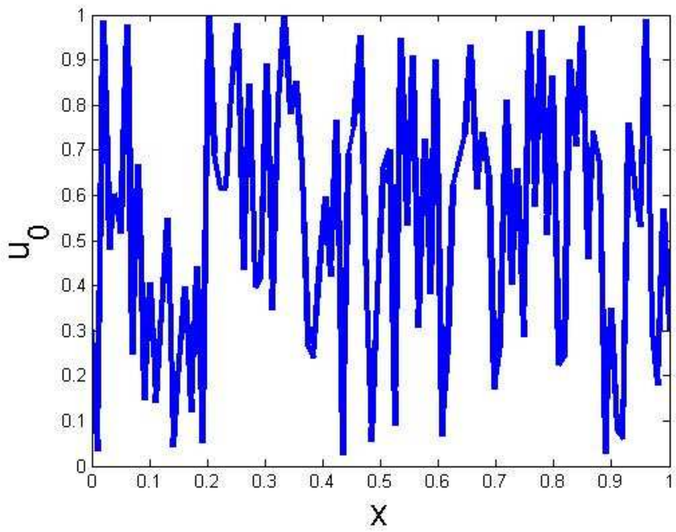
- Plot TKE versus time for different schemes

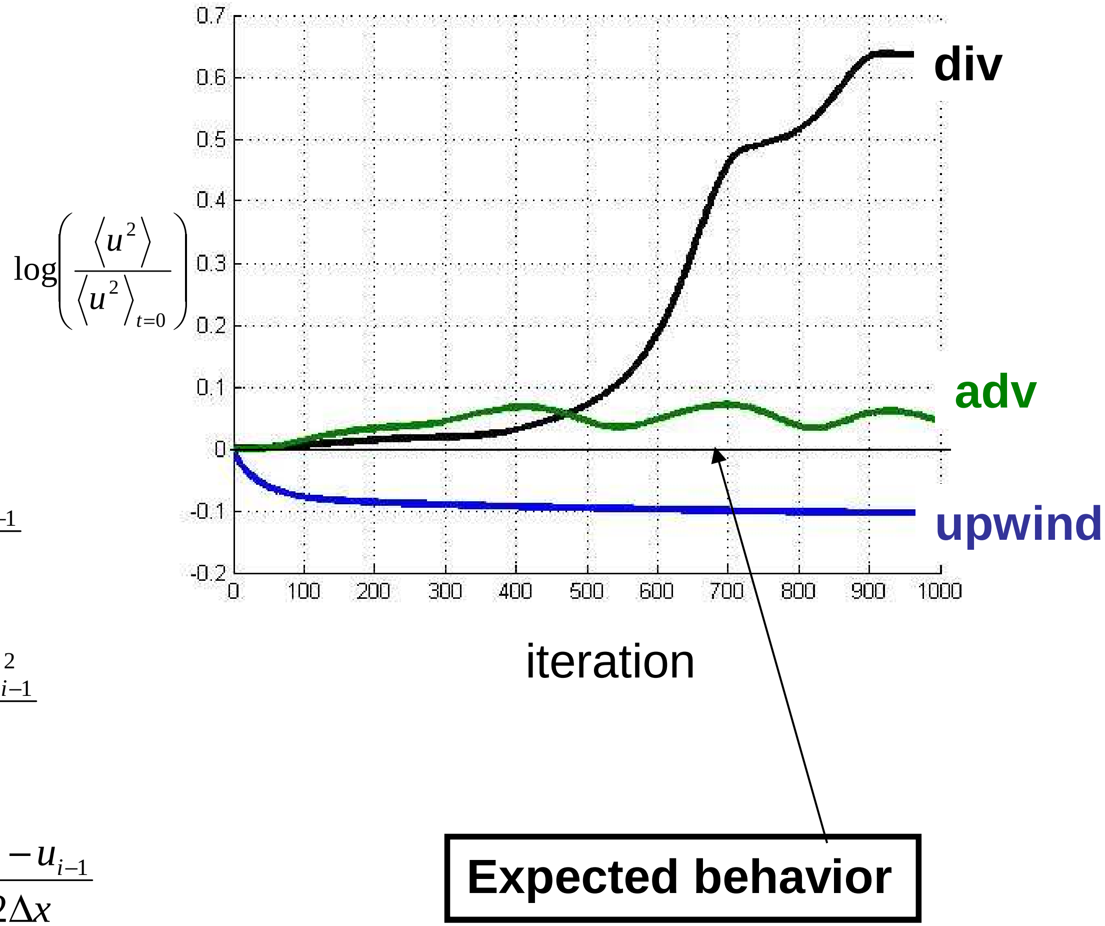
  - Upwind biased $$\frac{\partial u^2}{\partial x} \approx \frac{u_i^2 - u_{i-1}^2}{\Delta x}$$

  - Centered, divergence form $$\frac{\partial u^2}{\partial x} \approx \frac{u_{i+1}^2 - u_{i-1}^2}{2\Delta x}$$

  - Centered, advective form $$\frac{\partial u^2}{\partial x} \approx 2u_i \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

Numerical test



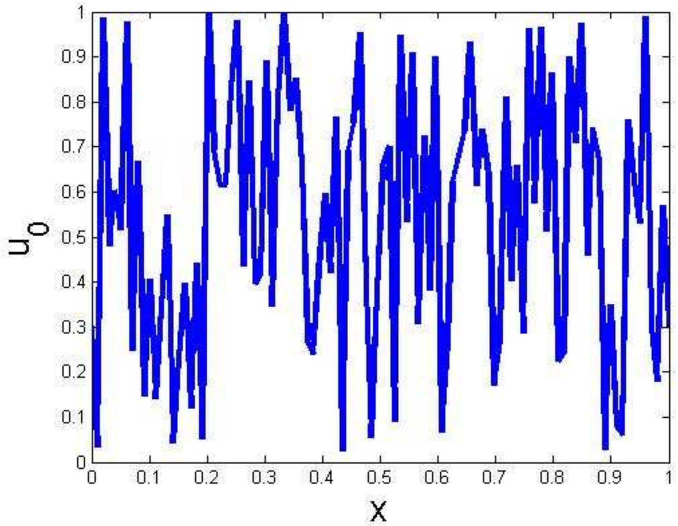


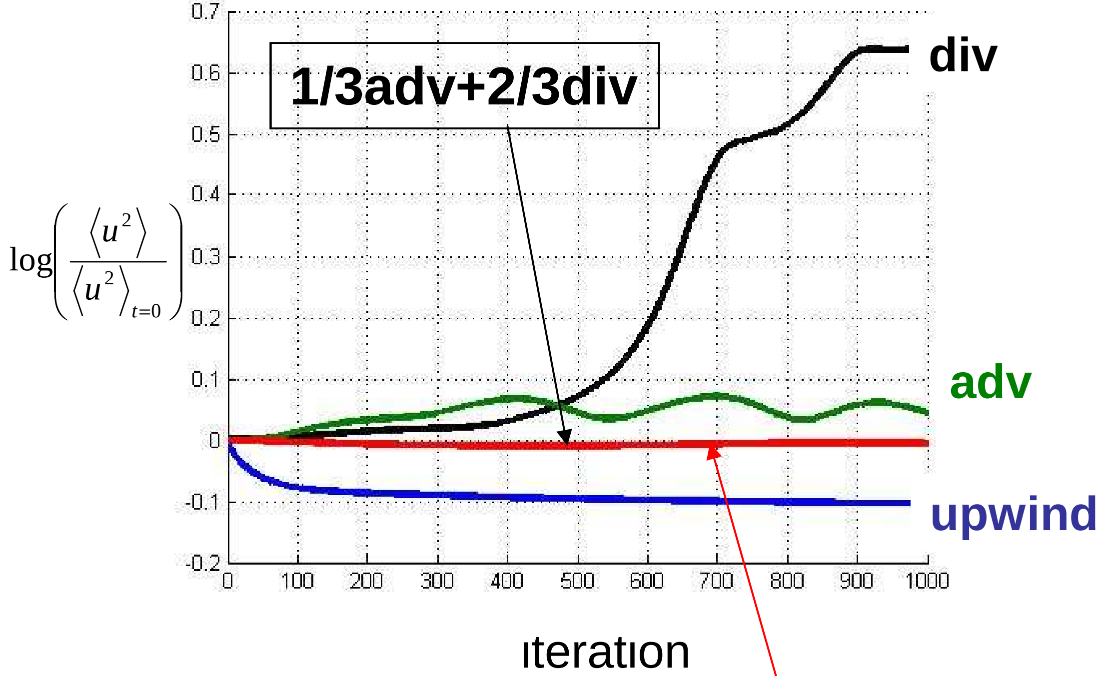
Upwind biased $\frac{\partial u^2}{\partial x} \approx \frac{u_i^2 - u_{i-1}^2}{\Delta x}$

Divergence form $\frac{\partial u^2}{\partial x} \approx \frac{u_{i+1}^2 - u_{i-1}^2}{2\Delta x}$

Advective form $\frac{\partial u^2}{\partial x} \approx 2u_i \frac{u_{i+1} - u_{i-1}}{2\Delta x}$

Numerical test





Centered, hybrid form:

$$\frac{\partial u^2}{\partial x} \approx \frac{1}{3}\left(2u_i \frac{u_{i+1} - u_{i-1}}{2\Delta x} + 2\frac{u_{i+1}^2 - u_{i-1}^2}{2\Delta x} \right)$$

Expected behavior obtained
by mixing adv and div

Explanation

Divergence form

$$\text{node } i: \quad u\frac{\partial u^2}{\partial x}dx \approx u_i \frac{u_{i+1}^2 - u_{i-1}^2}{2}$$

$$\text{node } i+1: \quad u\frac{\partial u^2}{\partial x}dx \approx u_{i+1} \frac{u_{i+2}^2 - u_{i}^2}{2}$$

$$\text{node } i+2: \quad u\frac{\partial u^2}{\partial x}dx \approx u_{i+2} \frac{u_{i+3}^2 - u_{i+1}^2}{2}$$

$$\ldots + \frac{u_i u_{i+1}^2 - u_i^2 u_{i+1}}{2} + \frac{u_{i+1} u_{i+2}^2 - u_{i+1}^2 u_{i+2}}{2} + \ldots$$

Advective form

$$\text{node } i: \quad 2u^2\frac{\partial u}{\partial x}dx \approx u_i^2 \left(u_{i+1} - u_{i-1}\right)$$

$$\text{node } i+1: \quad 2u^2\frac{\partial u}{\partial x}dx \approx u_{i+1}^2 \left(u_{i+2} - u_{i}\right)$$

$$\text{node } i+2: \quad 2u^2\frac{\partial u}{\partial x}dx \approx u_{i+2}^2 \left(u_{i+3} - u_{i+1}\right)$$

$$\ldots + u_i^2 u_{i+1} - u_i u_{i+1}^2 + u_{i+1}^2 u_{i+2} - u_{i+1} u_{i+2}^2 + \ldots$$

For *2 x Divergence form + Advective form*, the sum is zero …

$$\frac{\partial u^2}{\partial x} \approx \frac{1}{3}\left(2u_i \frac{u_{i+1} - u_{i-1}}{2\Delta x} + 2\frac{u_{i+1}^2 - u_{i-1}^2}{2\Delta x}\right)$$

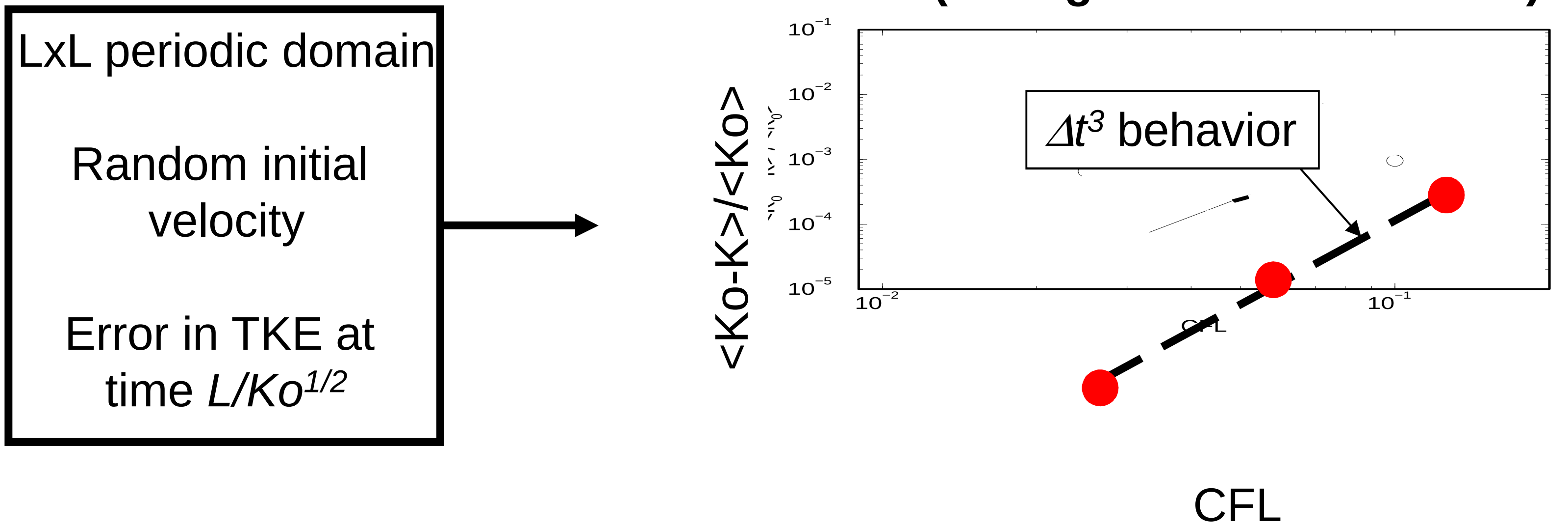
Generalization to Navier-Stokes

- The same strategy can be applied to Navier-Stokes,
- The convection term are then discretized under the

skew-symmetric form $\frac{1}{2}\left(\frac{\partial u_i u_j}{\partial x_j} + u_j \frac{\partial u_i}{\partial x_j}\right)$

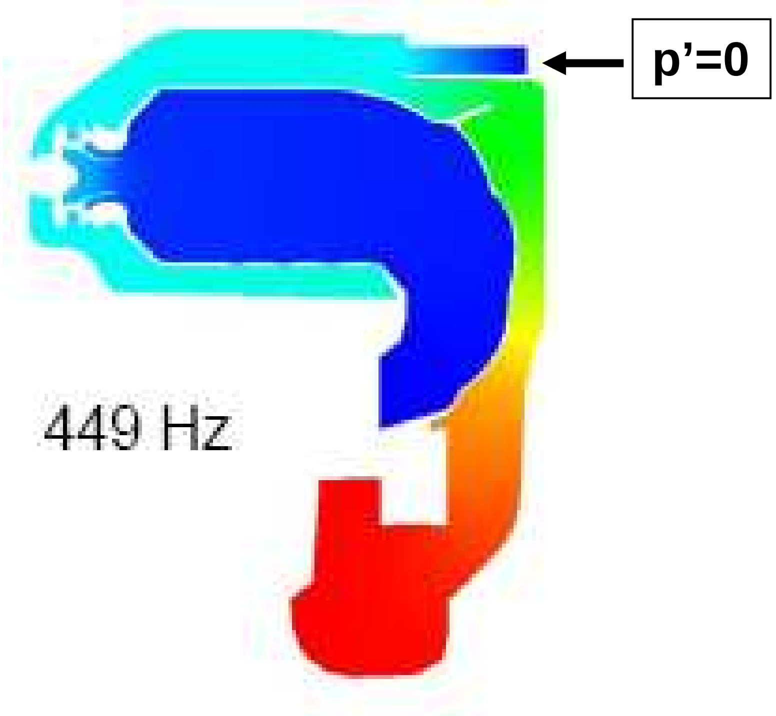
Conservative mixed scheme

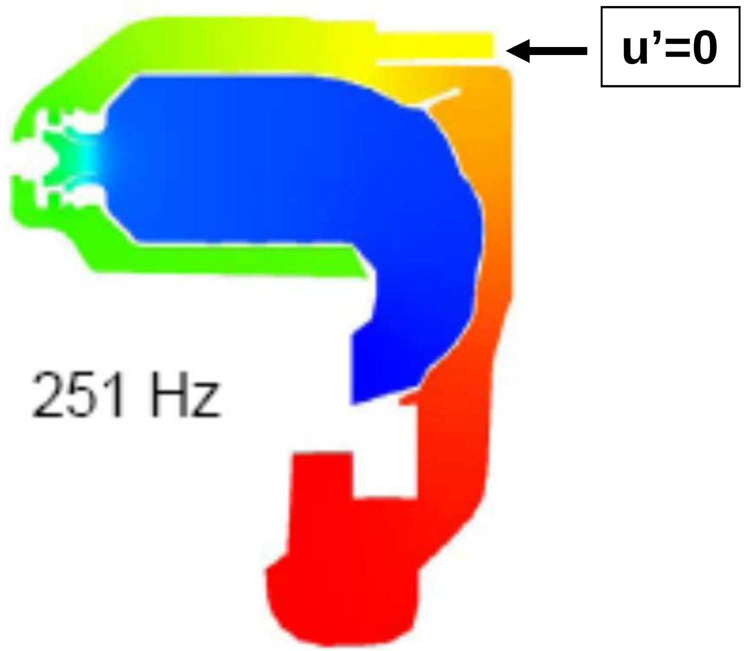
(Divergence form unstable)



Boundary conditions

BC essential for thermo-acoustics



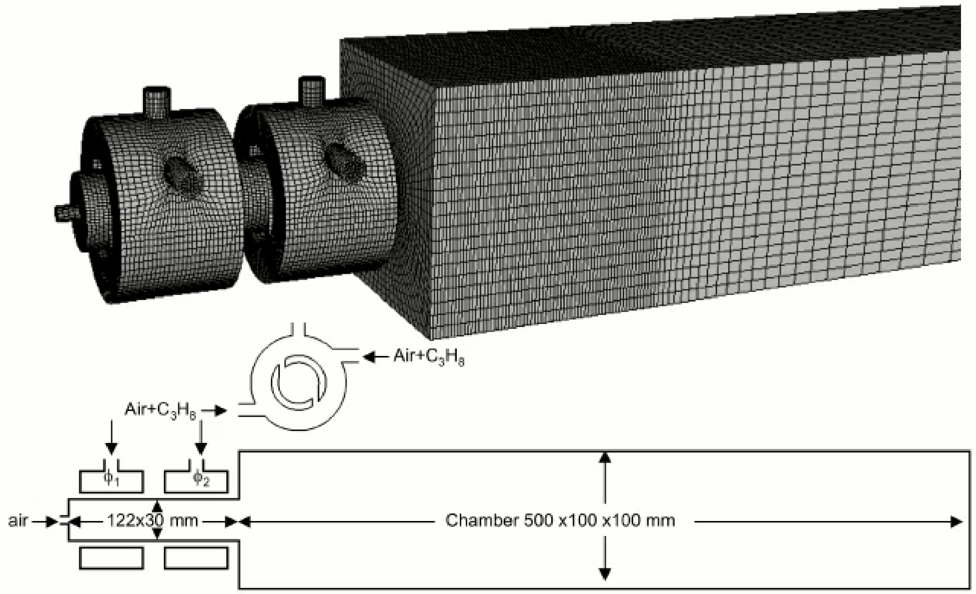


Acoustic analysis of a Turbomeca combustor including
the swirler, the casing and the combustion chamber
C. Sensiau (CERFACS/UM2) – AVSP code

BC essential for thermo-acoustics

ECP Mod Lab burner

Fully premixed propane injection
Stage 30%
Non reflecting inlets
Reflecting outlet from begining to t=0.1728s
Partially non reflecting outlet from t=0.1728s to the end
The movie presents iso-surface T=1500K colored by axial velocity
Chamber walls: pressure, injection pipe plan: axial velocity



C. Martin (CERFACS) – AVBP code

Numerical test

- 1D convection equation (*D=0*)

$$\frac{\partial f}{\partial t} + U_0 \frac{\partial f}{\partial x} = 0, \quad -8\,\mathrm{m} \le x \le 8\,\mathrm{m}, \quad U_0 = 1\,\mathrm{m/s}$$

- Initial and boundary conditions:

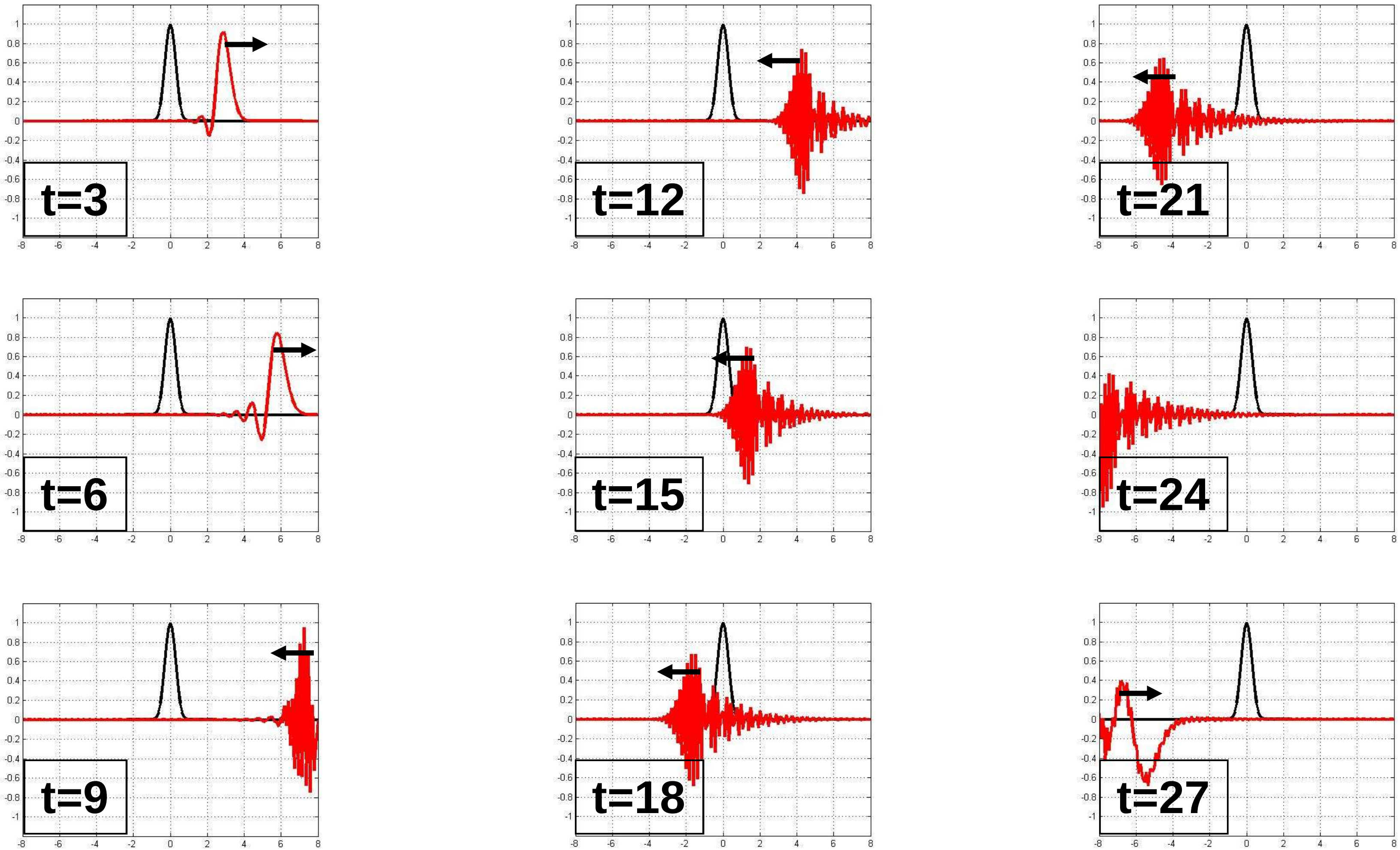
$f(-8,t) = 0$

$$f(x,0) = \exp\left(-x^2/4a^2\right), \quad a = 0.2\,\mathrm{m}$$

Zero order extrapolation

Numerical test

$$\frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} = 0$$



Basic Equations

Primitive form: Simpler for analytical work

The time dependent Navier-Stokes equations are hyperbolic, and can be reformulated in a set of characteristic advection equations. Let us consider the 3D Euler equations in quasi-linear form:

$$\frac{\partial \mathbf{V}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{V}}{\partial x} + \mathbf{B}\frac{\partial \mathbf{V}}{\partial y} + \mathbf{C}\frac{\partial \mathbf{V}}{\partial z} = \mathbf{AoT}$$

Not included in wave decomposition

In this equation, $\mathbf{V} = (\rho, u, v, w, P)^T$ is the vector of the primitive variables, the matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ gather the inviscid contributions and AoT stand for "all the other terms" (viscous terms and sources):

$$\mathbf{A} = \begin{bmatrix} u & \rho & . & . & . \\ . & u & . & . & 1/\rho \\ . & . & u & . & . \\ . & . & . & u & . \\ . & \gamma P & . & . & u \end{bmatrix} \mathbf{B} = \begin{bmatrix} v & . & \rho & . & . \\ . & v & . & . & . \\ . & . & v & . & 1/\rho \\ . & . & . & v & . \\ . & . & \gamma P & . & v \end{bmatrix} \mathbf{C} = \begin{bmatrix} w & . & . & \rho & . \\ . & w & . & . & . \\ . & . & w & . & . \\ . & . & . & w & 1/\rho \\ . & . & . & \gamma P & w \end{bmatrix},$$

where γ, ρ, $\vec{v} = (u, v, w)^T$ and P represent the isentropic coefficient, the density, the velocity vector and the static pressure respectively.

Decomposition in waves in 1D

- 1D Eqs: $\frac{\partial V}{\partial t} + A\frac{\partial V}{\partial x} = AoT$ $\quad A = \begin{bmatrix} u & \rho & . \\ . & u & 1/\rho \\ . & \gamma P & u \end{bmatrix}$

A can be diagonalized: ***A = L⁻¹Λ L***

$$L = \begin{bmatrix} 1 & 0 & -1/c^2 \\ 0 & 1 & 1/\rho c \\ 0 & -1 & 1/\rho c \end{bmatrix} \quad \Lambda = \begin{bmatrix} u & . & . \\ . & u+c & . \\ . & . & u-c \end{bmatrix} \quad L^{-1} = \begin{bmatrix} 1 & \rho/2c & \rho/2c \\ 0 & 1/2 & -1/2 \\ 0 & \rho c/2 & \rho c/2 \end{bmatrix}$$

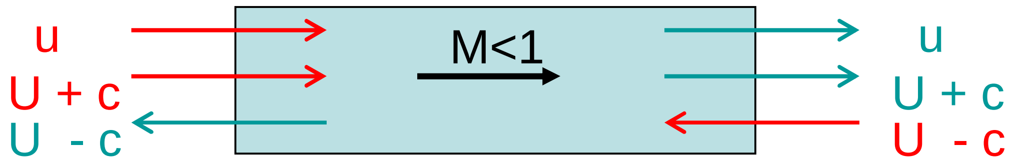
- Introducing the characteristic variables: $\delta W = L\delta V$

$$\delta W = \begin{bmatrix} \delta W^1 \\ \delta W^2 \\ \delta W^3 \end{bmatrix} = \begin{bmatrix} \delta\rho - \delta P/c^2 \\ \delta u + \frac{1}{\rho c}\delta P \\ -\delta u + \frac{1}{\rho c}\delta P \end{bmatrix} \begin{matrix} \rightarrow speed \quad u \quad [kg/m^3] \\ \rightarrow speed \quad u+c \quad [m/s] \\ \rightarrow speed \quad u-c \quad [m/s] \end{matrix}$$

- Multiplying the state Eq. by L: $\frac{\partial W}{\partial t} + \Lambda\frac{\partial W}{\partial x} = L.AoT$

Remarks

• δW^i with positive (resp. negative) speed of propagation may enter or leave the domain, depending on the boundary



• in 3D, the matrices A, B and C can be diagonalized BUT they have different eigenvectors, meaning that the definition of the characteristic variables is not unique.

Decomposition in waves: 3D

- Define a local orthonormal basis $\left(\vec{n}, \vec{t}_1, \vec{t}_2\right)$ with $\vec{n} = \left(n_x, n_y, n_z\right)$ the inward vector normal to the boundary

- Introduce the normal matrix : $E_n = n_x A + n_y B + n_z C$

- Define the characteristic variables by: $\delta W_n = L_n . \delta V$, $E_n = L_n^{-1} . \Lambda_n . L_n$

$$\Lambda_n = diag\left(u_n, u_n, u_n, u_n + c, u_n - c\right), \quad u_n = \vec{u} . \vec{n}$$

$$\begin{bmatrix} \delta\rho \\ \delta u \\ \delta v \\ \delta w \\ \delta P \end{bmatrix} = \begin{bmatrix} \delta W_n^1 + \frac{\rho}{2c}(\delta W_n^4 + \delta W_n^5) \\ s_{1x}\delta W_n^2 + s_{2x}\delta W_n^3 + \frac{n_x}{2}(\delta W_n^4 - \delta W_n^5) \\ s_{1y}\delta W_n^2 + s_{2y}\delta W_n^3 + \frac{n_y}{2}(\delta W_n^4 - \delta W_n^5) \\ s_{1z}\delta W_n^2 + s_{2z}\delta W_n^3 + \frac{n_z}{2}(\delta W_n^4 - \delta W_n^5) \\ \frac{\rho c}{2}(\delta W_n^4 + \delta W_n^5) \end{bmatrix}$$

$$\delta \mathbf{W_n} = \begin{bmatrix} \delta W_n^1 \\ \delta W_n^2 \\ \delta W_n^3 \\ \delta W_n^4 \\ \delta W_n^5 \end{bmatrix} = \begin{bmatrix} \delta\rho - \frac{1}{c^2}\delta P \\ \vec{t_1}.\delta\vec{u} \\ \vec{t_2}.\delta\vec{u} \\ +\vec{n}.\delta\vec{u} + \frac{1}{\rho c}\delta P \\ -\vec{n}.\delta\vec{u} + \frac{1}{\rho c}\delta P \end{bmatrix} \begin{matrix} \to u_n \\ \to u_n \\ \to u_n \\ \to u_n + c \\ \to u_n - c \end{matrix}$$

Which wave is doing what ?

WAVE	SPEED	INLET ($u_n > 0$)	OUTLET ($u_n < 0$)
δW_n^1 entropy	u_n	in	out
δW_n^2 shear	u_n	in	out
δW_n^3 shear	u_n	in	out
δW_n^4 acoustic	$u_n + c$	in	in
δW_n^5 acoustic	$u_n - c$	out	out

General implementation

- Compute the predicted variation of V as given by the scheme of integration with all physical terms without boundary conditions.

  Note δV^{P} this predicted variation.

- Estimate the ingoing wave(s) and remove its (their) contribution(s).

  Note $\delta V^{out} = \delta V^{P} - L^{-1}\delta W^{in}$ the remaining variation.

- Assess the corrected ingoing wave(s) $\delta W^{in,C}$ depending on the physical condition at the boundary. Note $\delta V^{in} = L^{-1}.\delta W^{in,C}$ its (their) contribution.

- Compute the corrected variation of the solution during the iteration as:

$$\delta V^{C} = \delta V^{out} + \delta V^{in} = \delta V^{P} - L^{-1}.\delta W^{in} + L^{-1}.\delta W^{in,C}$$

Pressure imposed outlet

- Compute the predicted value of δP, viz. δP^P, and decompose it into waves:

$$\delta P^P = \frac{\rho c}{2}\left(\delta W_n^4 + \delta W_n^5\right)$$

- δW_n^4 is entering the domain; the contribution of the outgoing wave reads:

$$\delta P^{out} = \frac{\rho c}{2}\left(\delta W_n^5\right)$$

- The corrected value of δW_n^4 is computed through the relation:

$$\delta W_n^{4,C} = -\delta W_n^5 + \frac{2}{\rho c}\boxed{\delta P^t}$$

Desired pressure variation at the boundary

- The final (corrected) update of P is then:

$$\boxed{\delta P^C} = \delta P^{out} + \delta P^{in,C} = \frac{\rho c}{2}\left(\delta W_n^5 + \delta W_n^{4,C}\right) = \boxed{\delta P^t}$$

OK !

Defining waves: non-reflecting BC

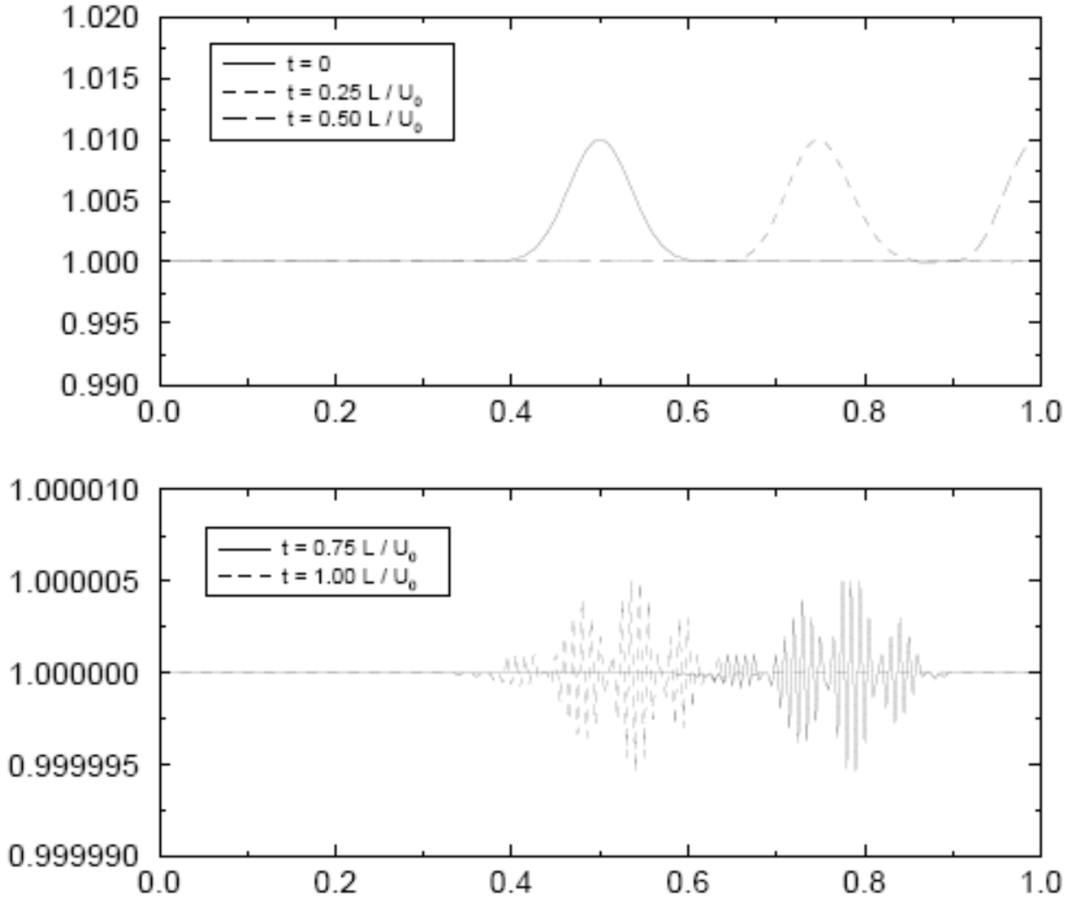
- Very simple in principle: $\delta W_n^4 = 0$

- « Normal derivative » approach: $$-(u_n - c)\frac{\partial W_n^4}{\partial n}\Delta t = 0$$

- « Full residual » approach: $$\frac{\partial W_n^4}{\partial t}\Delta t = 0$$

- No theory to guide our choice … Numerical tests required

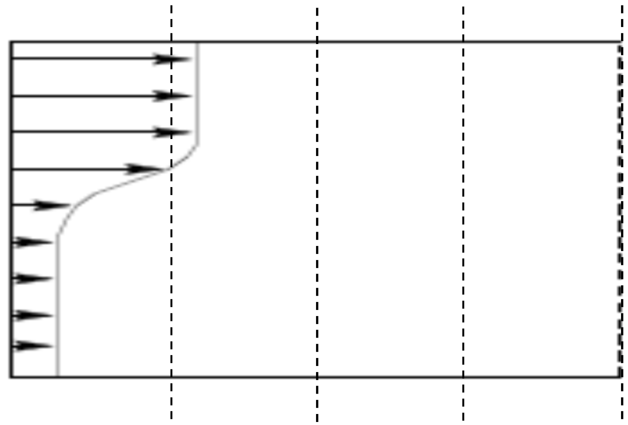
1D entropy wave



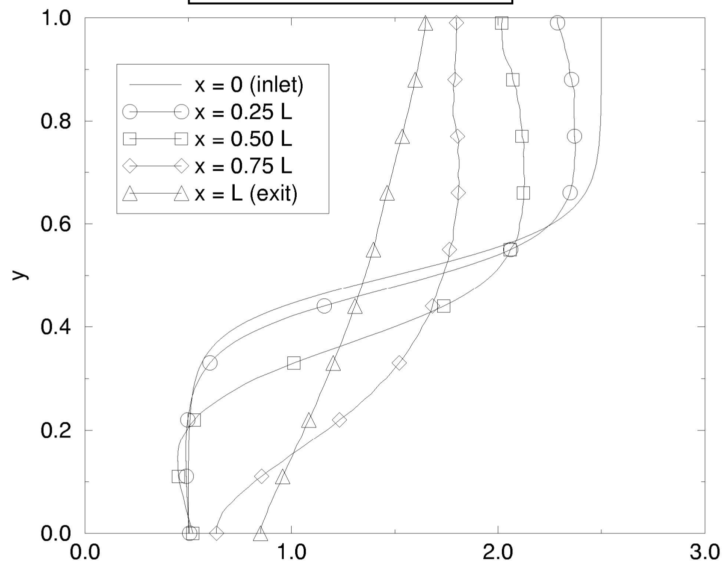
Same result with both the "normal derivative" and the "full residual" approaches

2D test case

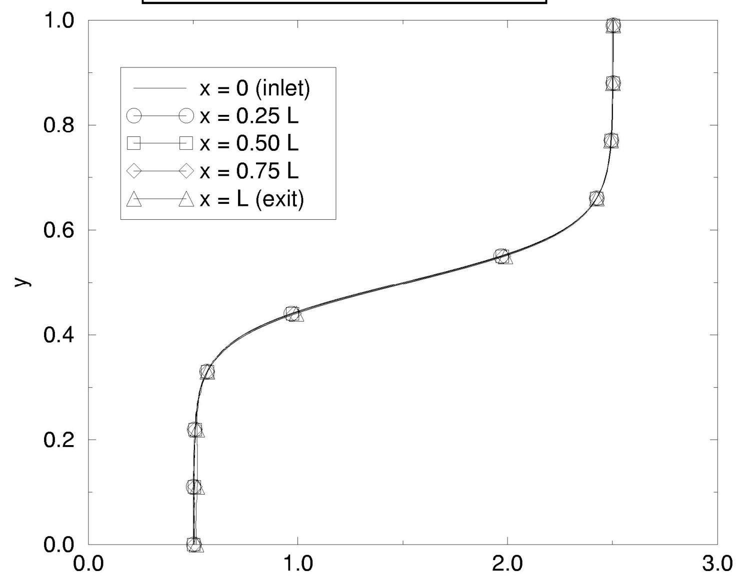
- A simple case: 2D inviscid shear layer with zero velocity and constant pressure at t=0



Full residual



Normal residual



Outlet with relaxation on P

- Start from $\delta W_n^4 = -\delta W_n^5 + \frac{2}{\rho c}\delta P$

- Cut the link between ingoing and outgoing waves to make the condition non-reflecting $\delta W_n^4 = +\frac{2}{\rho c}\delta P$

- Set $\delta P = \alpha_P \left(P^t - P^B\right)\Delta t$ to relax the pressure at the boundary towards the target value P^t

- To avoid over-relaxation, $\alpha_P \Delta t$ should be less than unity. $\alpha_P \Delta t = 0$ means 'perfectly non-reflecting' (ill posed)

Inlet with relaxation on velocity and Temperature

- Cut the link between ingoing and outgoing waves
- Set $\delta V = \alpha\left(V^t - V^B\right)\Delta t$ to drive V^B towards V^t
- Use either the normal or the full residual approach

to compute the waves and correct the ingoing ones via:

$$\begin{bmatrix} \delta W_n^1 \\ \delta W_n^2 \\ \delta W_n^3 \\ \delta W_n^4 \end{bmatrix} = \begin{bmatrix} \frac{(\gamma-1)\rho}{c^2}\left[-C_p\alpha_T(T^t - T^B) + c\alpha_{u_n}(u_n^t - u_n^B)\right]\Delta t \\ \alpha_{u_t}(u_{t_1}^t - u_{t_1}^B)\Delta t \\ \alpha_{u_t}(u_{t_2}^t - u_{t_2}^B)\Delta t \\ 2\alpha_{u_n}(u_n^t - u_n^B)\Delta t \end{bmatrix}$$

Integral boundary condition

- in some situations, the target value is not known pointwise. E.g.: the outlet pressure of a swirled flow

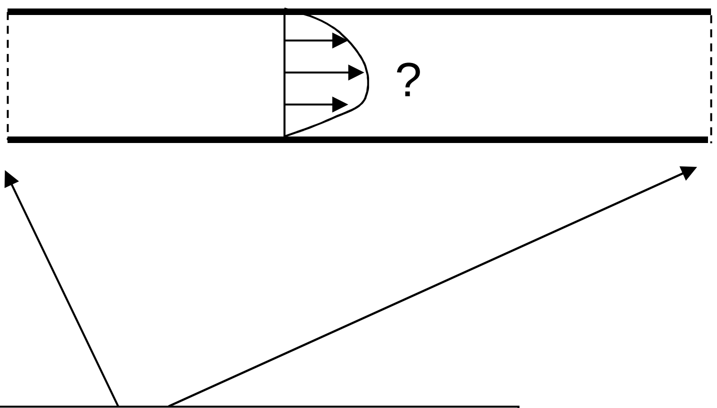
- use the relaxation BC framework

- rely on integral values to generate the relaxation term to avoid disturbing the natural solution at the boundary

$$\delta V = \alpha \Delta t \left(V^{t}_{\mathrm{bulk}} - \frac{1}{S_{\mathrm{Boundary}}} \int_{\mathrm{Boundary}} V^{B} dS \right)$$

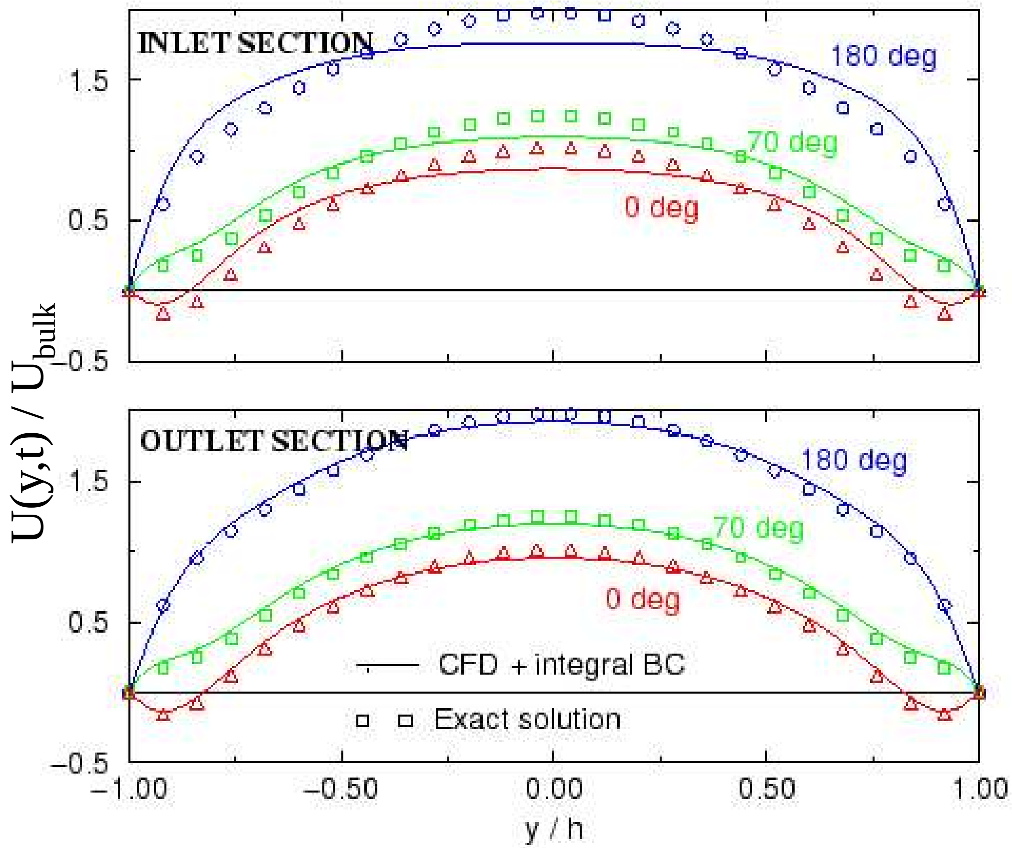
Integral boundary condition

- periodic pulsated channel flow (laminar)

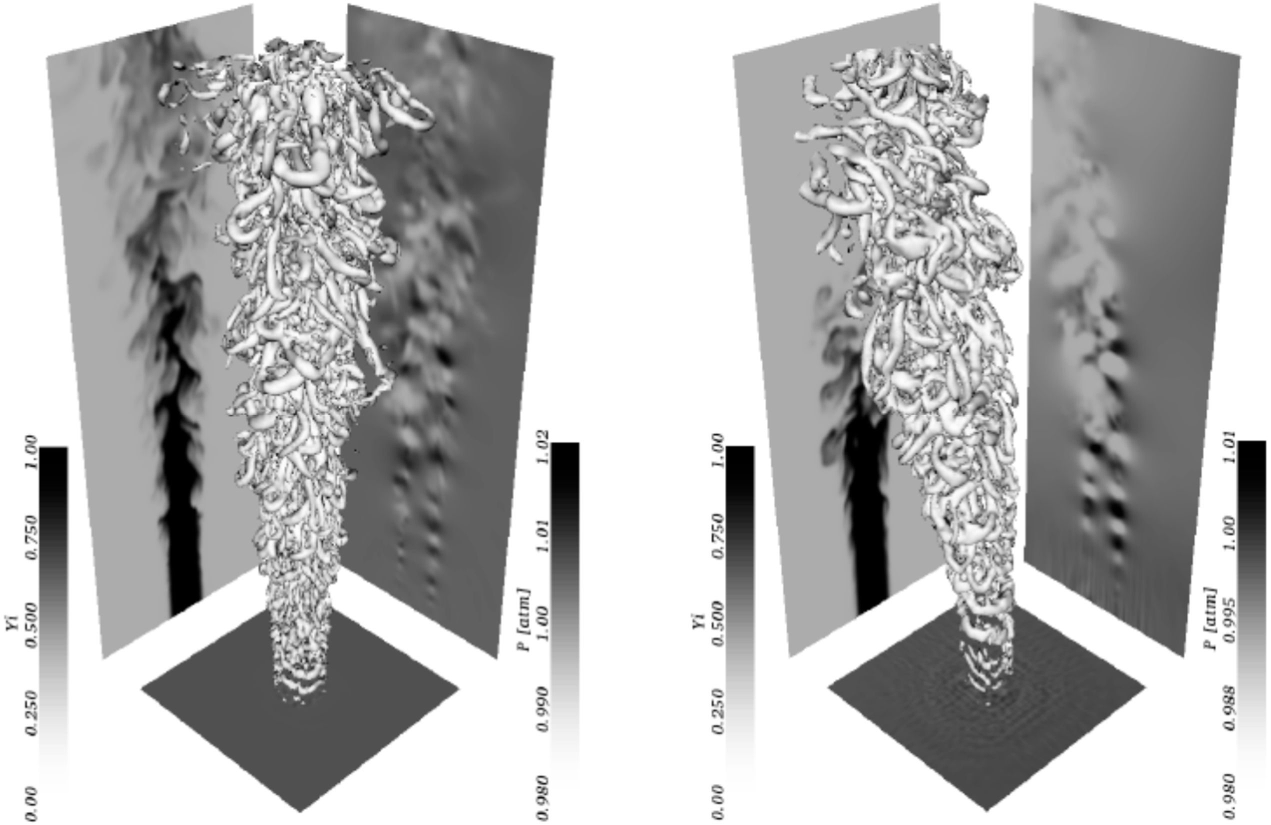


Integral BCs to impose the flow rate

$$u^t_{\text{bulk}} = u_0 + u_1 \sin(\omega t)$$



Everything is in the details



Lodato, Domingo and Vervish – CORIA Rouen

THANK YOU

More details, slides, papers, …

http://www.math.univ-montp2.fr/~nicoud/