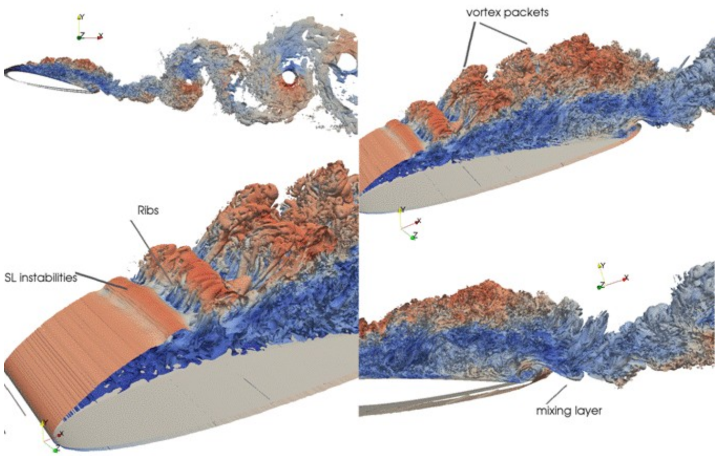
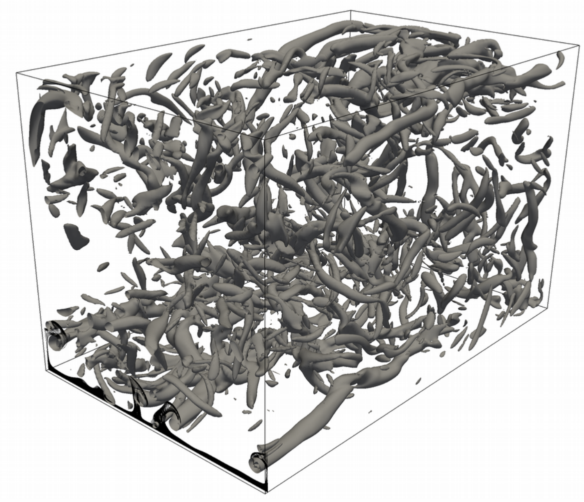
# DISCRETE PHYSICAL REALM

ALGEBRAIC FORMULATION OF PHYSICS

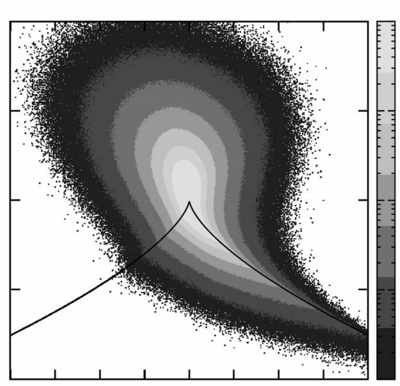
A. BÁEZ, F.X. TRIAS AND N. VALLE

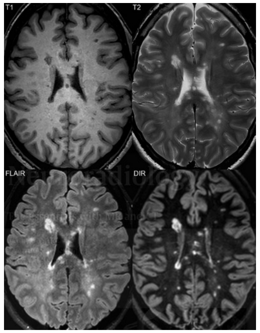


# INVARIANTS

## FLOW TOPOLOGY, VISUALIZATION AND TURBULENCE MODELING






*“ First, solve the problem. Then, write the code. ” John Johnson*

# WHAT IS AN INVARIANT?

**Def**: an invariant is a property, held by a class of mathematical objects, which **remains unchanged** when transformations of a certain type are applied to the objects. Namely,

Given an isomorphism $T: U \rightarrow U$

$I(x)$ is an invariant respect to $T \quad \Leftrightarrow \quad I(T(x)) = I(x), \forall x \in U$

| $U$ | $I(x)$ | $T: U \rightarrow U$ |
|---|---|---|
| $\mathbb{R}^n$ | Euclidean distance between 2 points | {Space translations; Rotations; Reflexions;...} |
| $\mathbb{R}^{n \times n}$ | {Determinant; Trace; Eigenvalues; Eigenvectors; conditioning number;...} | Changes of basis |
| $\mathbb{C}$ | $\mathbb{R}(x)$ | $\mathbb{R}(\overline{x}) = \mathbb{R}(x)$ |

# TENSOR INVARIANTS: THEORY

Let us consider a $3\times3$ tensor: $\boldsymbol{A}\in\mathbb{R}^{3\times3}$

Three eigenvalues of $\boldsymbol{A}$: $\lambda_1\geq\lambda_2\geq\lambda_3$

They are solutions of the characteristic equation:

$$det(\lambda \boldsymbol{I}-\boldsymbol{A})=\lambda^3-P\lambda^2+Q\lambda-R=0$$

$$P=\lambda_1+\lambda_2+\lambda_3$$ ← First invariant

$$Q=\lambda_1\lambda_2+\lambda_1\lambda_3+\lambda_2\lambda_3$$ ← Second invariant

$$R=\lambda_1\lambda_2\lambda_3$$ ← Third invariant

# TENSOR INVARIANTS: THEORY

Caley-Hamilton theorem:

$$\lambda^3 - P\lambda^2 + Q\lambda - R = 0 \quad \Rightarrow \quad \boldsymbol{A}^3 - P\boldsymbol{A}^2 + Q\boldsymbol{A} - R\boldsymbol{I} = \boldsymbol{0}$$

Trace: $tr(\boldsymbol{A}^3) - P\,tr(\boldsymbol{A}^2) + Q\,tr(\boldsymbol{A}) - 3R = 0$

$$P = tr(\boldsymbol{A})$$

First invariant

$$Q = \frac{1}{2}\left(tr^2(\boldsymbol{A}) - tr(\boldsymbol{A}^2)\right)$$

Second invariant

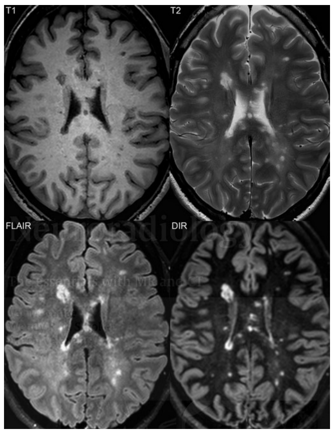
$$R = det(\boldsymbol{A}) = \frac{1}{6}\left(tr^3(\boldsymbol{A}) - 3\,tr(\boldsymbol{A})\,tr(\boldsymbol{A}^2) + 2\,tr(\boldsymbol{A}^3)\right)$$

Third invariant

# TENSOR INVARIANTS: THEORY

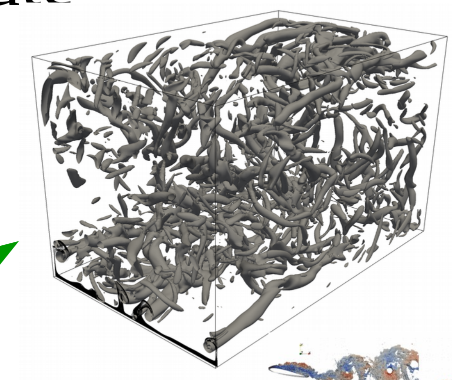
$$\{\lambda_1, \lambda_2, \lambda_3\} \Leftrightarrow \{P, Q, R\} \Leftrightarrow \{tr(\boldsymbol{A}), tr(\boldsymbol{A}^2), tr(\boldsymbol{A}^3)\}$$

$P, Q$ and $R$ have a clear physical meaning and they are easier to compute



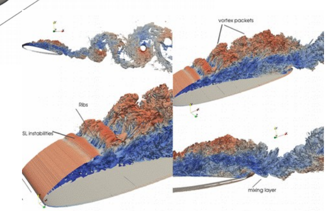

MRI

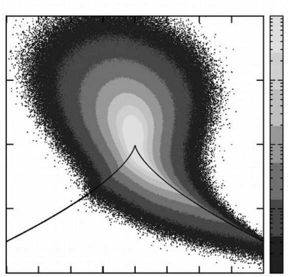
Flow visualization



$$\{P, Q, R\}$$

Turbulence modeling





Flow topology analysis

$$\nu_e^{Smag} = (C_s \Delta)^2 |S(\bar{u})| = 2 (C_s \Delta)^2 \sqrt{-Q_S}$$

# MORE THEORY: INDEX NOTATION

$$a_{ij}=[\boldsymbol{A}]_{ij} \qquad b_{ij}=[\boldsymbol{B}]_{ij} \qquad c_{ij}=[\boldsymbol{C}]_{ij}$$

**To know this is a MUST!**

*Products:*

$$[\boldsymbol{AB}]_{ik}=a_{ij}b_{jk} \qquad [\boldsymbol{AB}^T]_{ik}=a_{ij}b_{kj} \qquad [\boldsymbol{ABC}]_{ik}=a_{ij}b_{jk}c_{km}$$

*Tensor contraction (trace):*

$$tr(\boldsymbol{A})=a_{ii} \qquad tr(\boldsymbol{AB})=a_{ij}b_{ji} \qquad tr(\boldsymbol{ABC})=a_{ij}b_{jk}c_{ki}$$

So easy to show that $tr(\boldsymbol{ABC})=tr(\boldsymbol{BCA})=tr(\boldsymbol{CAB})$

$$a_{ij}b_{jk}c_{ki}=b_{ij}c_{jk}a_{ki}=c_{ij}a_{jk}b_{ki}$$

Kronecker delta: $\delta_{ij}=\begin{cases} 0 & i\neq j \\ 1 & i=j \end{cases}$ Levi-Civita tensor: $\epsilon_{ijk}=\begin{cases} 1 \\ -1 \\ 0 \end{cases}$

$$\boldsymbol{e}_i\boldsymbol{e}_j=\delta_{ij} \qquad [\nabla\times\boldsymbol{a}]_k=\epsilon_{ijk}\partial_i a_j \qquad [\boldsymbol{a}\times\boldsymbol{b}]_k=\epsilon_{ijk}a_i b_j$$

$$\nabla \cdot \boldsymbol{a} = \partial_i a_i \qquad \nabla \boldsymbol{a} = \partial_i a_j \qquad \nabla^2 \boldsymbol{a} = \partial_{ii} a_j$$

**To know this is a MUST!**

It is easier to prove vector calculus identities, e.g.

$$\nabla \cdot (\nabla \boldsymbol{a})^T = \nabla \nabla \cdot \boldsymbol{a} \longrightarrow \partial_i \partial_j a_i = \partial_j \partial_i a_i$$

$$\nabla \times \nabla \varphi = 0 \longrightarrow \epsilon_{ijk} \partial_i \partial_j \varphi = \epsilon_{jik} \partial_i \partial_j \varphi = 0$$

$$\nabla \cdot \nabla \times \boldsymbol{a} = 0 \longrightarrow \partial_k \epsilon_{ijk} \partial_i a_j = \epsilon_{ijk} \partial_k \partial_i a_j = \epsilon_{jik} \partial_k \partial_i a_j = 0$$

$$\nabla \times \nabla^2 \boldsymbol{a} = \nabla^2 \nabla \times \boldsymbol{a} \longrightarrow \epsilon_{ijk} \partial_i \partial_{nn} a_j = \partial_{nn} \epsilon_{ijk} \partial_i a_j$$

# VELOCITY GRADIENT TENSOR

$$\boxed{\boldsymbol{G} \equiv \nabla \vec{u}}$$

Rate-of-strain tensor

$$\boldsymbol{S} = \frac{1}{2}\left(\boldsymbol{G} + \boldsymbol{G}^T\right)$$

Rate-of-rotation tensor

$$\boldsymbol{\Omega} = \frac{1}{2}\left(\boldsymbol{G} - \boldsymbol{G}^T\right)$$

$$P_G = tr(\boldsymbol{G}) = \nabla \cdot \vec{u} = 0 \qquad P_S = tr(\boldsymbol{S}) = 0 \qquad P_\Omega = tr(\boldsymbol{\Omega}) = 0$$

$$Q_G = -\frac{1}{2} tr\left(\boldsymbol{G}^2\right) \qquad Q_S = -\frac{1}{2} tr\left(\boldsymbol{S}^2\right) \qquad Q_\Omega = -\frac{1}{2} tr\left(\boldsymbol{\Omega}^2\right)$$

$$R_G = \frac{1}{3} tr\left(\boldsymbol{G}^3\right) \qquad R_S = \frac{1}{3} tr\left(\boldsymbol{S}^3\right) \qquad R_\Omega = \frac{1}{3} tr\left(\boldsymbol{\Omega}^3\right)$$

$$tr\left(\boldsymbol{S}^2\right) = S_{ij} S_{ji} = S_{ij} S_{ij} \longrightarrow Q_S = -1/2\left(\boldsymbol{S} : \boldsymbol{S}\right) \leq 0 \longleftrightarrow \varepsilon = 2 \nu \boldsymbol{S} : \boldsymbol{S}$$

$$tr\left(\boldsymbol{\Omega}^2\right) = \Omega_{ij} \Omega_{ji} = -\Omega_{ij} \Omega_{ij} \longrightarrow Q_\Omega = 1/2\left(\boldsymbol{\Omega} : \boldsymbol{\Omega}\right) = 1/2 \left|\vec{\omega}\right|^2 \geq 0$$

$$tr\left(\boldsymbol{S\Omega}\right) = S_{ij} \Omega_{ji} = -S_{ji} \Omega_{ij} = 0 \longrightarrow \boxed{Q_G = Q_S + Q_\Omega}$$

# FLOW TOPOLOGY & VISUALIZATION

$$\boxed{G \equiv \nabla \vec{u}}$$

Rate-of-strain tensor

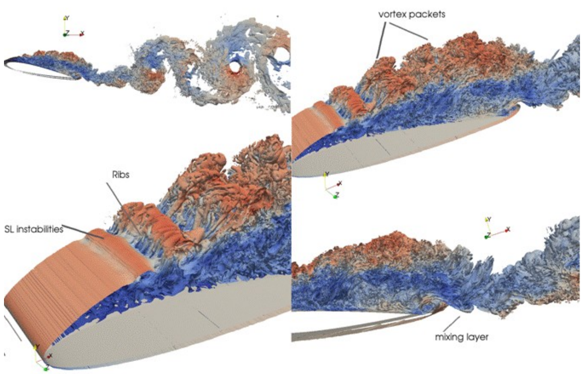
$$S = \frac{1}{2}\left(G + G^T\right)$$

Rate-of-rotation tensor

$$\Omega = \frac{1}{2}\left(G - G^T\right)$$

$$Q_S = -1/2\left(S : S\right) \leq 0 \longleftrightarrow \varepsilon = 2\nu S : S$$

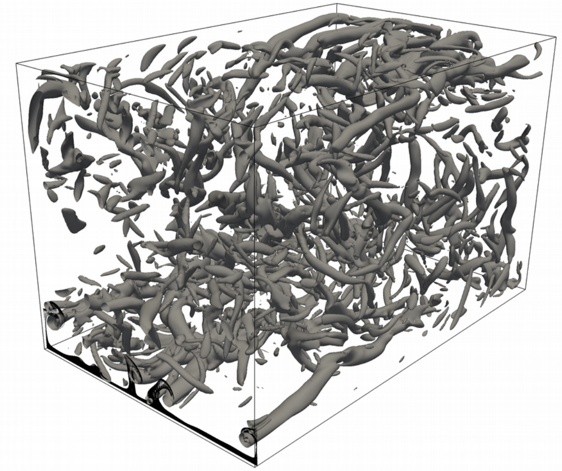
$$Q_\Omega = 1/2\left(\Omega : \Omega\right) = 1/2|\vec{\omega}|^2 \geq 0$$




$$\boxed{Q_G = Q_S + Q_\Omega}$$

$$Q_G > 0$$

**Tube-like structures!**



**Remark**: this is the well-known Q-criterion for flow visualization

$$\boxed{G \equiv \nabla \vec{u}}$$

$$\boxed{Q_G = Q_S + Q_\Omega}$$

$$\lambda^3 + Q\lambda - R = 0$$

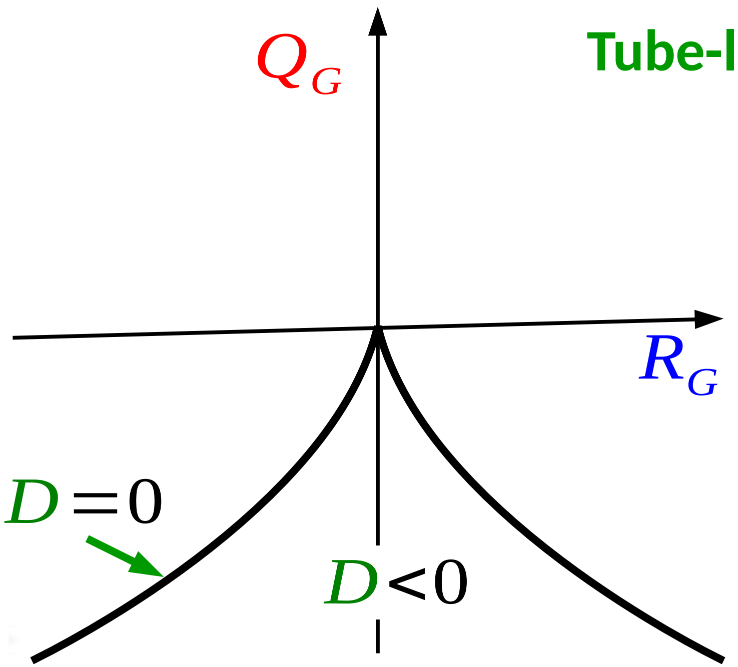
$$R = \lambda_1 \lambda_2 \lambda_3$$

$$D = (27/4) R^2 + Q^3$$

Discriminant

$$Q_G > 0$$

Tube-like structures!




$$D<0 \Rightarrow \lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$$

$$D>0 \Rightarrow \lambda_1 \in \mathbb{R}, \; \lambda_2 = \overline{\lambda_3} \in \mathbb{C}$$

Vortex!

$$D>0, R>0 \Rightarrow \lambda_1 > 0$$ vortex stretching

$$D>0, R<0 \Rightarrow \lambda_1 < 0$$ vortex compression

# FLOW TOPOLOGY & VISUALIZATION

**In these figures**

$$\lambda^3 + Q\lambda + R = 0$$
$$R = -\lambda_1 \lambda_2 \lambda_3$$

**...instead of**

$$\lambda^3 + Q\lambda - R = 0$$
$$R = \lambda_1 \lambda_2 \lambda_3$$

Flow dynamics for Restricted Euler equations (inviscid and no pressure)

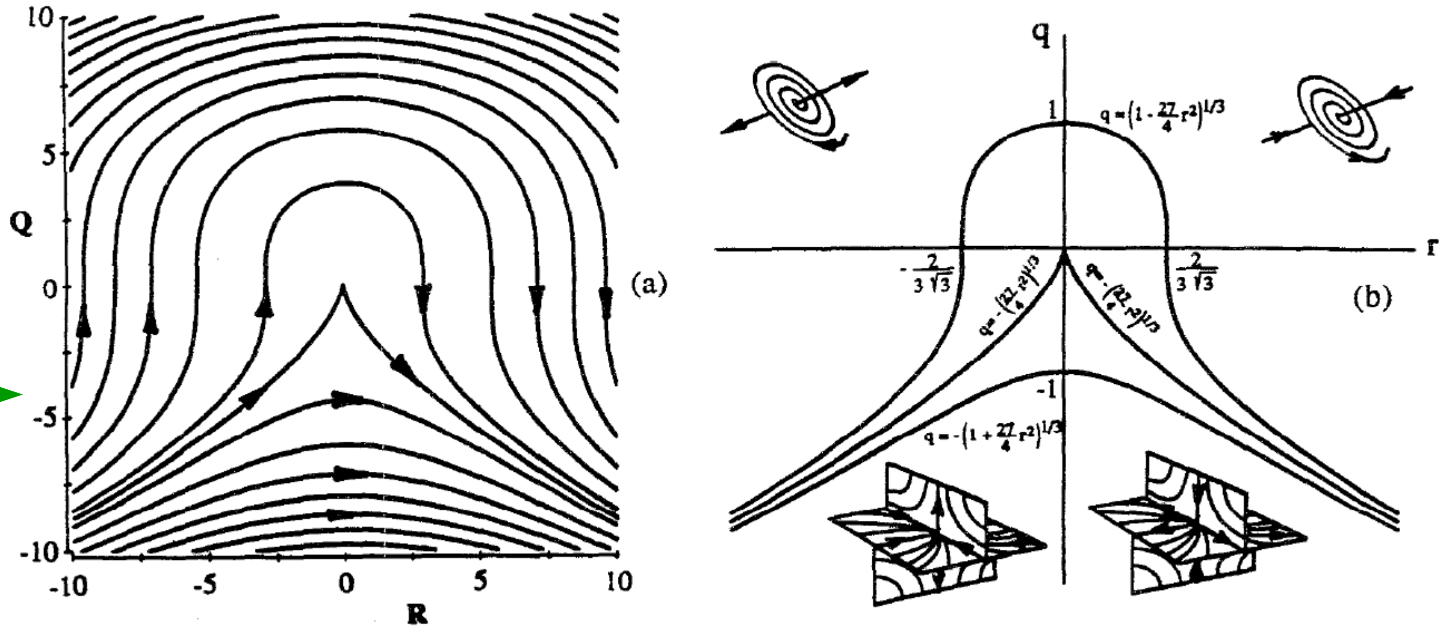



FIG. 1. Trajectories of the invariants of the velocity gradient tensor: (a) dimensioned $Q$ vs $R$, (b) dimensionless $q$ vs $r$ with schematic diagrams of local streamlines.

Figure extracted from: B. J. Cantwell, "Exact solution of the restricted Euler equation for the velocity gradient tensor," Phys. FluidsA4, 782 (1992).

**In these figures**

$$\lambda^3 + {\color{red}Q}\lambda + {\color{blue}R} = 0$$

$${\color{blue}R} = -\lambda_1 \lambda_2 \lambda_3$$

**...instead of**

$$\lambda^3 + {\color{red}Q}\lambda - {\color{blue}R} = 0$$

$${\color{blue}R} = \lambda_1 \lambda_2 \lambda_3$$

Flow dynamics for NS equations

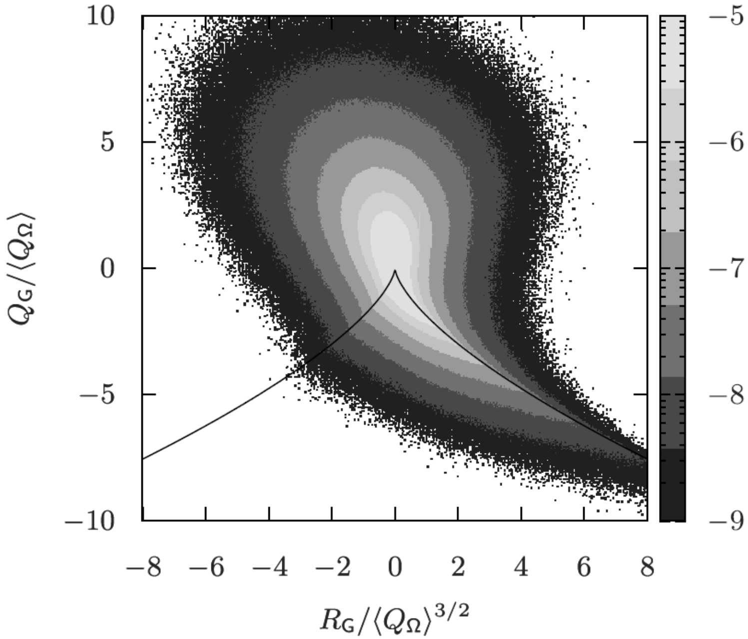



Figure extracted from: F. Dabbagh, F.X. Trias, A. Gorobets, and A. Oliva. "On the evolution of flow topology in turbulent Rayleigh-Bénard convection", Physics of Fluids, 28:115105, 2016.

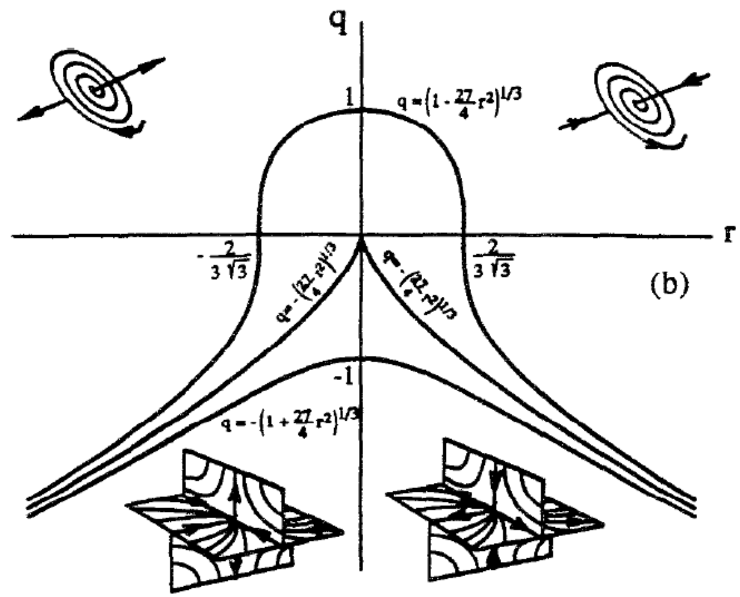
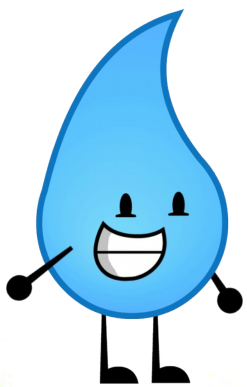
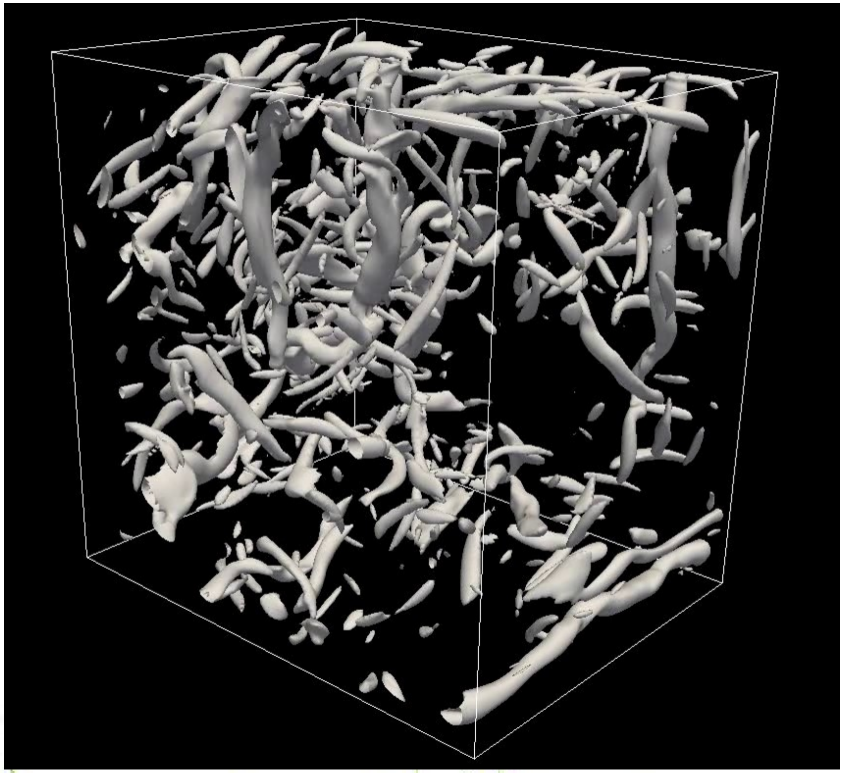


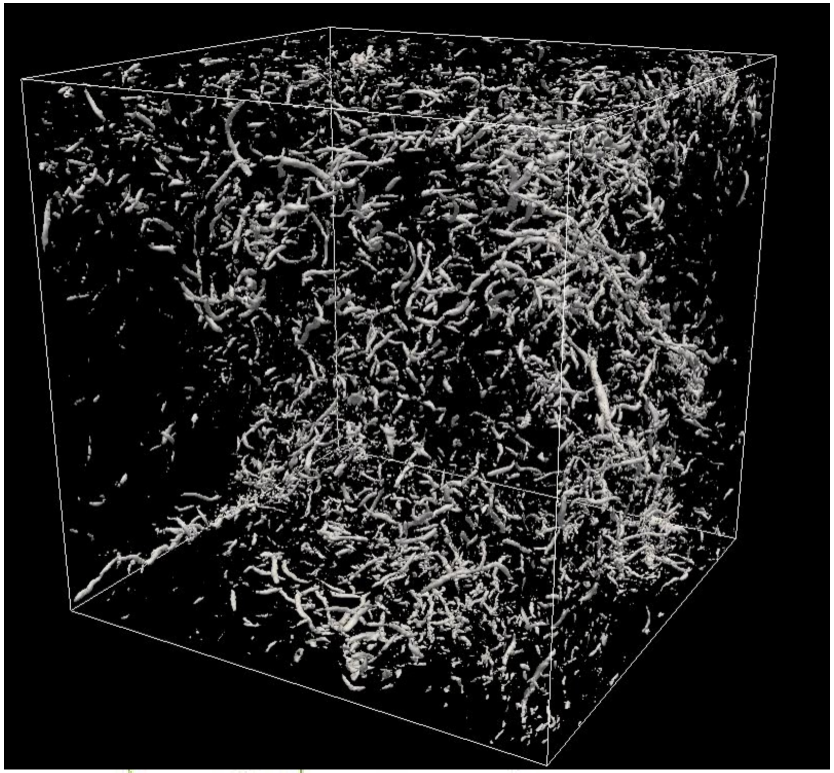

Figure extracted from: B. J. Cantwell, "Exact solution of the restricted Euler equation for the velocity gradient tensor," Phys. FluidsA4, 782 (1992).



$$\boxed{Q_G = Q_S + Q_\Omega}$$

$Q_G > 0$ **Tube-like structures!**





$$V^2 = |S\vec{\omega}|^2 \qquad \boxed{\{Q_G, R_G, Q_S, R_S, V^2\}} \longleftarrow \textbf{Unified framework!}$$

**Smagorinsky (1963)**
J. Smagorinsky, Mon. Weather Rev. 91, 99–164 (1963)

$$\longrightarrow \nu_e^{Smag} = (C_S\Delta)^2 |S(\bar{u})| = 2(C_S\Delta)^2(-Q_S)^{1/2}$$

**WALE (1999)**
F. Nicoud and F. Ducros, Flow, Turbul. Combust. 62(3), 183-200 (1999)

$$\longrightarrow \nu_e^{W} = (C_W\Delta)^2 \frac{(V^2 + 2Q_G^2/3)^{3/2}}{(-2Q_S)^{5/2} + (V^2/2 + 2Q_G^2/3)^{5/4}}$$

**Vreman's (2004)**
A.W. Vreman, Phys. Fluids 16(10), 3670–3681 (2004)

$$\longrightarrow \nu_e^{Vr} = (C_{Vr}\Delta)^2 \left( \frac{V^2 + Q_G^2}{2(Q_G - 2Q_S)} \right)^{1/2}$$

**QR-model (2011)**
R. Verstappen, J. Sci. Comput. 49(1), 94–110 (2011)

$$\longrightarrow \nu_e^{Ve} = (C_{Ve}\Delta)^2 \frac{|R_S|}{-Q_S}$$

**Sigma (2011)**
F. Nicoud et al.," Phys. Fluids 23(8), 085106 (2011)

$$\longrightarrow \nu_e^{\sigma} = (C_\sigma\Delta)^2 \frac{\sigma_3(\sigma_1 - \sigma_2)(\sigma_2 - \sigma_3)}{\sigma_1^2}; \quad \sigma_i = \sqrt{\lambda_i^{GG^T}}$$

**S3QR (2015)**
F.X.Trias et al. Phys. Fluids, 27: 065103, (2015)

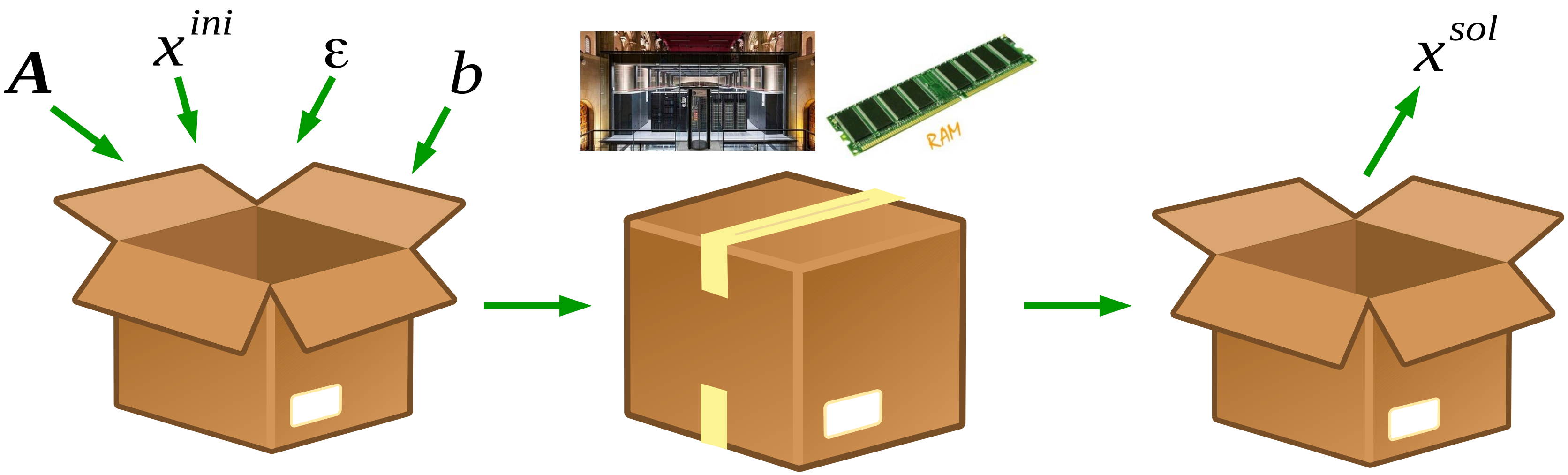
$$\longrightarrow \nu_e^{S3QR} = (C_{S3QR}\Delta)^2 \frac{R_G^{5/3}}{Q_G - 2Q_S}$$

# DISCRETE PHYSICAL REALM

ALGEBRAIC FORMULATION OF PHYSICS

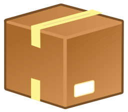
# BONUS: LINEAR SOLVERS

$$\boxed{\boldsymbol{A}x=b} \longrightarrow x^{sol} \approx \boldsymbol{A}^{-1}b \quad \text{where } \|\boldsymbol{A}x^{sol}-b\| \leq \varepsilon$$



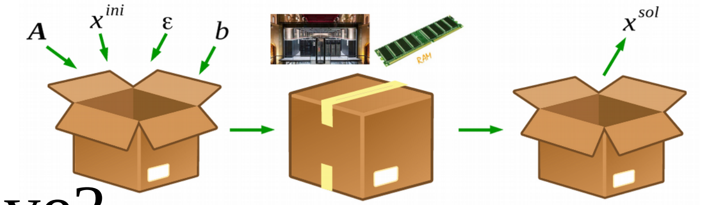

Easy to test!

$$x^{rand} \longrightarrow b=\boldsymbol{A}x^{rand} \xrightarrow[\varepsilon]{\boldsymbol{A}}$$



$$\longrightarrow x^{sol} \longrightarrow x^{sol} \approx x^{rand} \; ?$$

$$\boxed{\boldsymbol{A}x = b} \longrightarrow x^{sol} \approx \boldsymbol{A}^{-1} b \quad \text{where } \|\boldsymbol{A}x^{sol} - b\| \leq \varepsilon$$




How to choose a solver?

- What type of matrix/problem do I have?
  dense or sparse? $\boldsymbol{A} = \boldsymbol{A}^T$? diagonal dominant?...
  circulant? block diagonal? condition number?...
  $\boldsymbol{A}x_i = b_i$, $i = 1 \ldots N$; Is $N$ large or small?
- What is $\varepsilon$?
  do I need machine accuracy or $\varepsilon = 0.001$ is enough?
- How are $x^{ini}$ and $b$?
  is $x^{ini}$ a good guess of $x^{sol}$? what is the spectrum of $b$?
- How is my computer?
  parallel? memory shared or distributed?

# BONUS: LINEAR SOLVERS



Typical linear solvers in CFD:

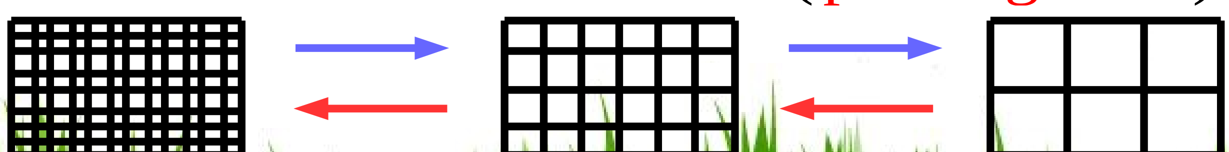
**To know this is a MUST!**

**Direct**

- Diagonalizable:
  - *e.g.* circulant matrix (easily solved with a FFT )
- LU-based: $\boldsymbol{A}x=\boldsymbol{L}\boldsymbol{U}x=b \;\Rightarrow\; y=\boldsymbol{L}^{-1}b \;\Rightarrow\; x=\boldsymbol{U}^{-1}y$
  - *e.g.* TDMA, band-LU, Cholesky (if $\boldsymbol{A}=\boldsymbol{A}^T$), Schur complement (for block/partitioned $\boldsymbol{A}$)

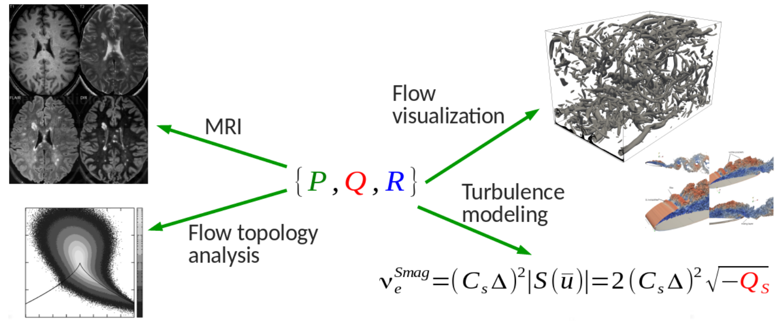
**Iterative**

- Stationary: $\boldsymbol{A}=\widetilde{\boldsymbol{A}}+(\boldsymbol{A}-\widetilde{\boldsymbol{A}}) \;\Rightarrow\; \widetilde{\boldsymbol{A}}x_{i+1}=b-(\boldsymbol{A}-\widetilde{\boldsymbol{A}})x_i$
  - *e.g.* Jacobi ($\widetilde{\boldsymbol{A}}=\boldsymbol{D}$), Gauss-Seidel ($\widetilde{\boldsymbol{A}}=\boldsymbol{D}+\boldsymbol{L}$), ...
- Non-stationary: *e.g.* Krylov subspace (CG if $\boldsymbol{A}=\boldsymbol{A}^T$), Multigrid solvers:
  - Smoother (e.g. Jacobi) easily solves high freqs
  - Idea: transform low freqs into high freqs (restriction) solve them and come back (prolongation)



# Take-away messages

- **Invariants** play a very important role in CFD: *e.g.* flow visualization (Q-criterion), turbulence modeling, flow topology analysis...

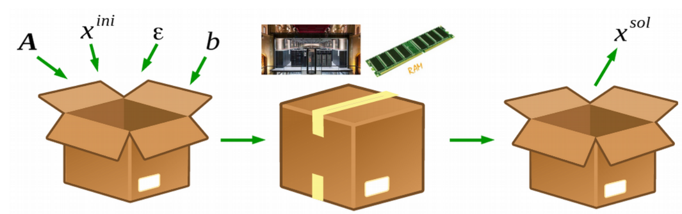



- (Sparse) **linear algebra** forms the lowest level of a CFD code. Hence, **few highly optimized basic operators** can be the basis of your code.

$y \leftarrow Ax;$ **SpMV**

$\alpha \leftarrow x \cdot y;$ **dot**

$y \leftarrow \alpha x + y$ **axpy**



# Open questions