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Nonlinear Wave Theory for Transport Phenomena

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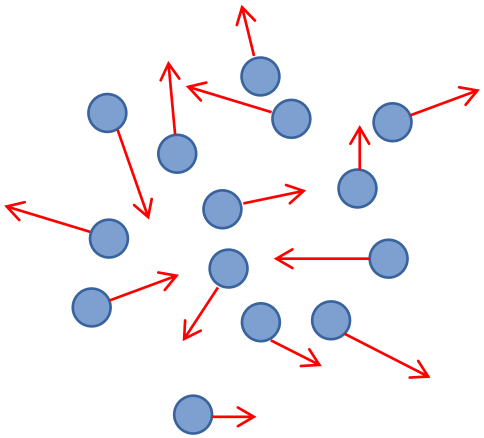
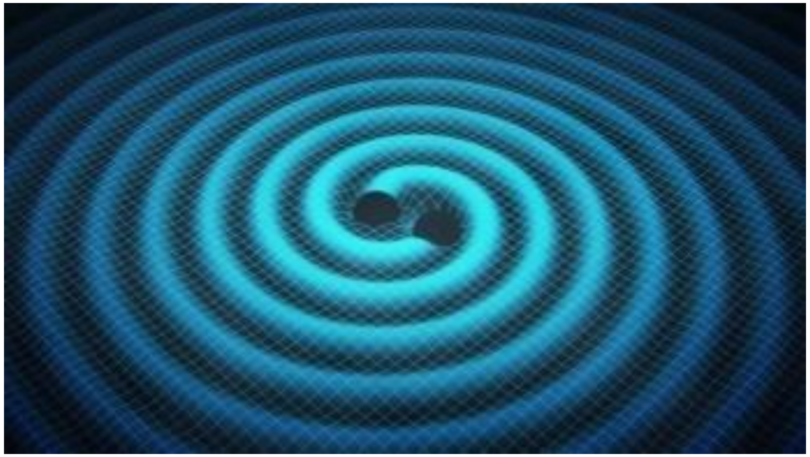
Motivation for a New Fluid Dynamics



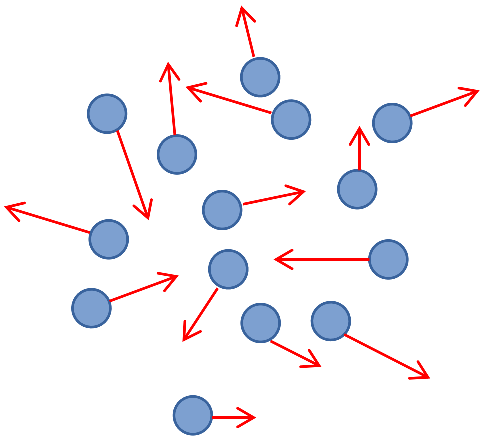
micro



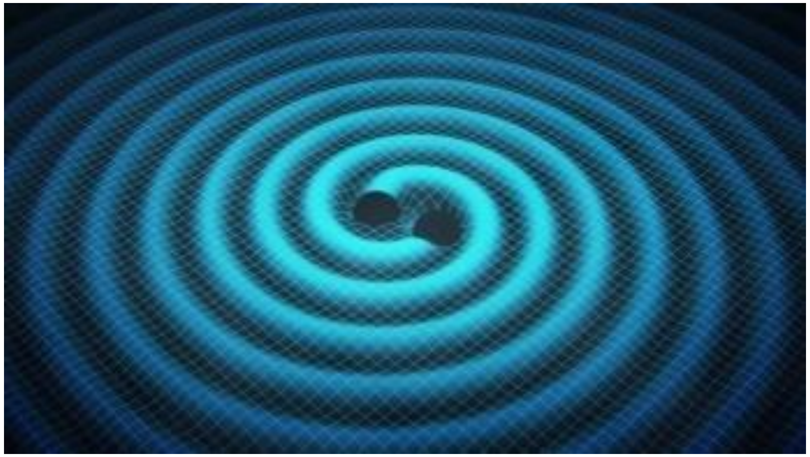
macro

Motivation for a New Fluid Dynamics

micro



macro



Classical **parabolic** transport theories (Navier-Stokes, Fourier, Fick) **are not "wave" theories** in a rigorous sense.

Classical **Kirchhoff** equation (dispersion relation for NS) says that at **high** frequencies

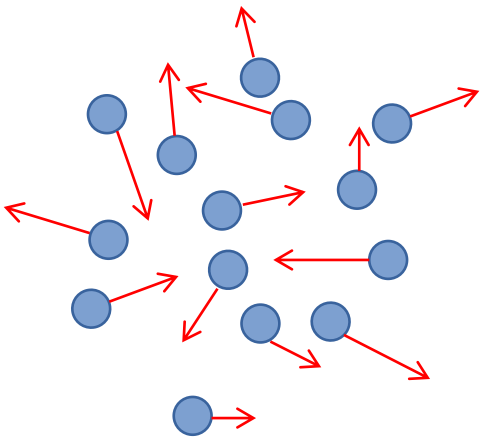
$$V \approx \omega^{1/2}$$

Unified hyperbolic model for fluids and solids

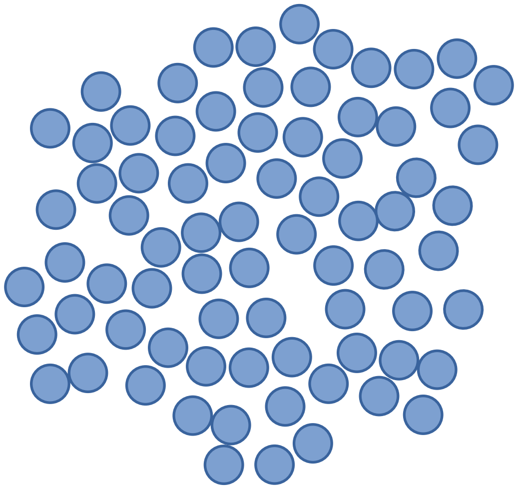
- First order **Hyperbolic** model (genuinely wave theory)
- Can describe **fluids and solids** in a one system of PDEs
- **Free of empirical steady-state** transport relations (Newton's law of viscosity, Fourier heat conduction law etc.)
- Applicable to **non-Newtonian, non-Fourier, non-Fickian** transport
- **Has less numerical issues** than parabolic theory (mesh quality, discontinuities, singularities)

Continuum mechanics

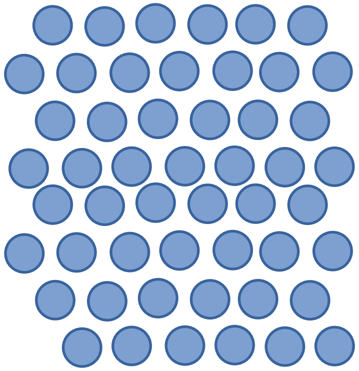
Gas



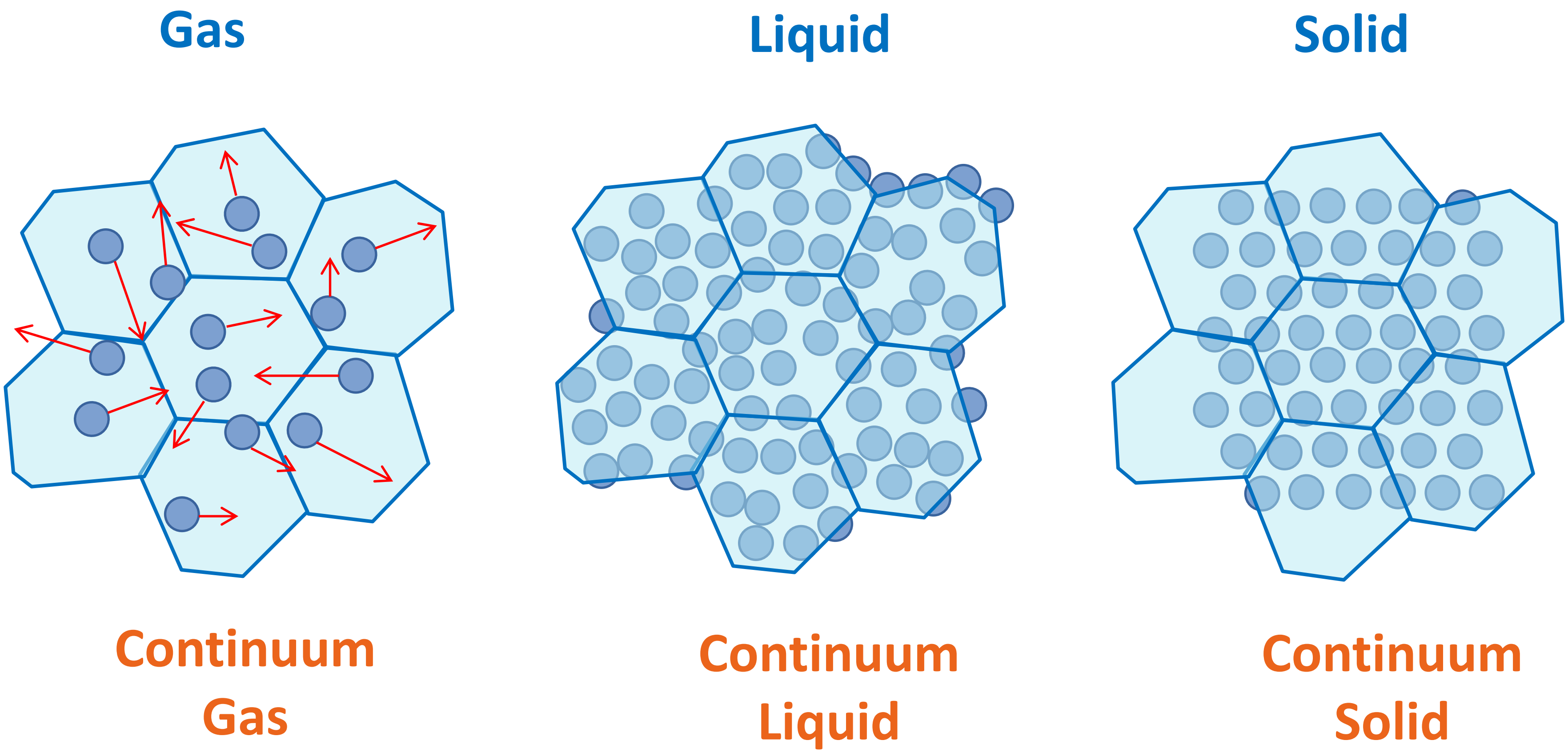
Liquid



Solid

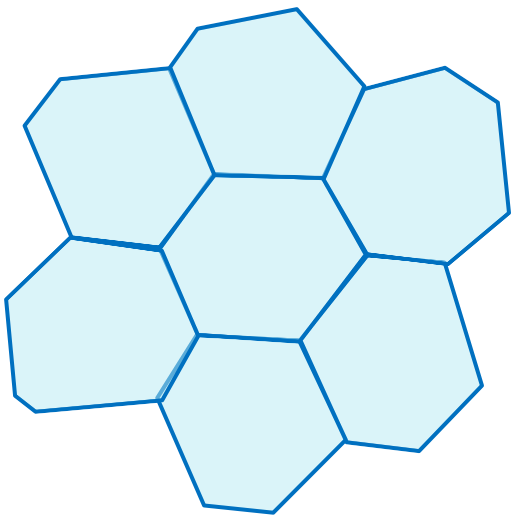


Continuum mechanics



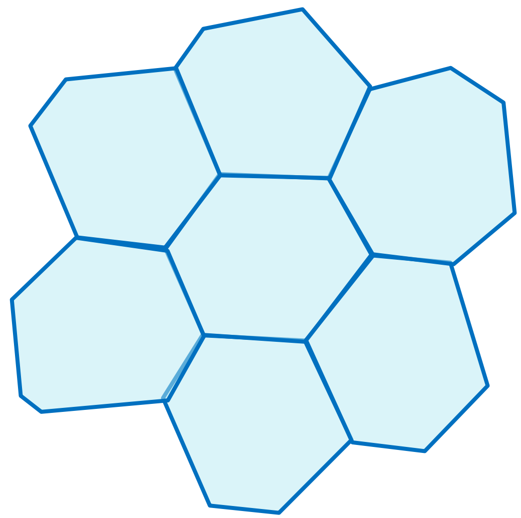
Continuum mechanics

Gas



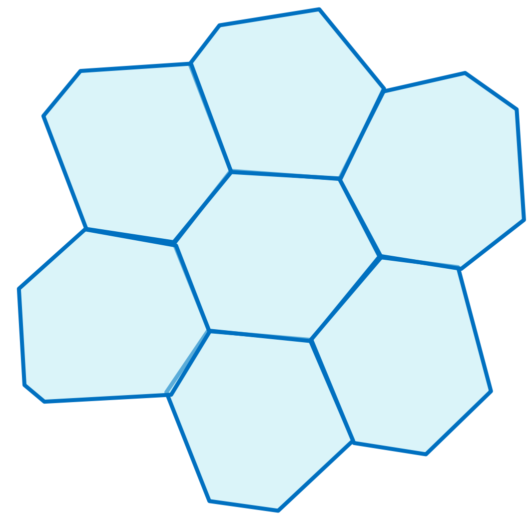
Continuum
Gas

Liquid



Continuum
Liquid

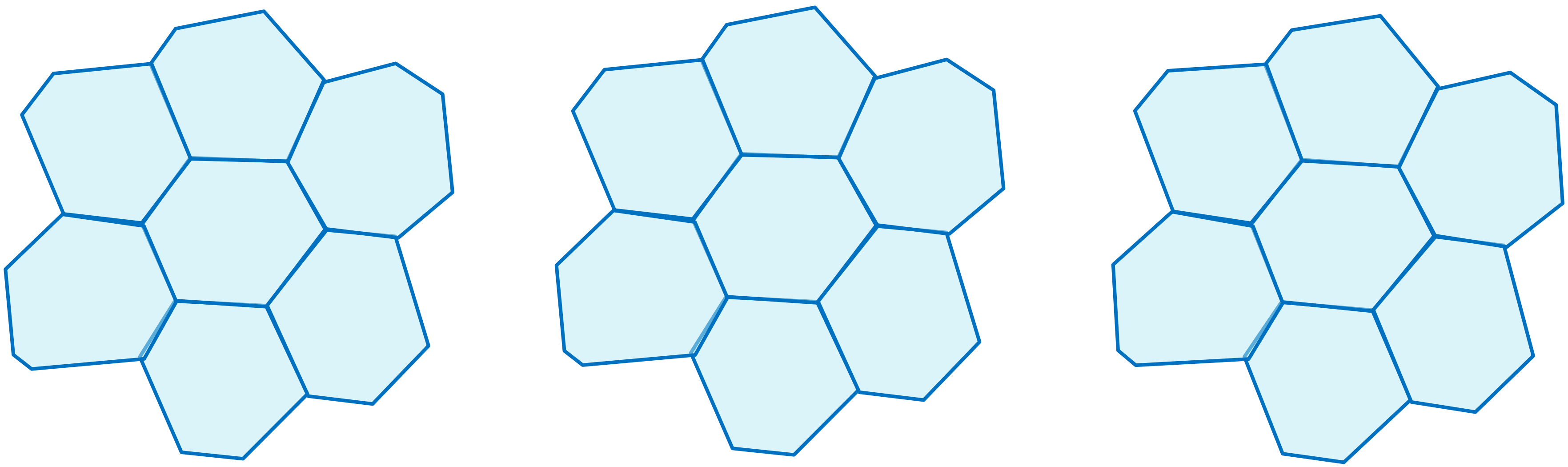
Solid



Continuum
Solid

Continuum mechanics

Gas **Liquid** **Solid**



Continuum Gas

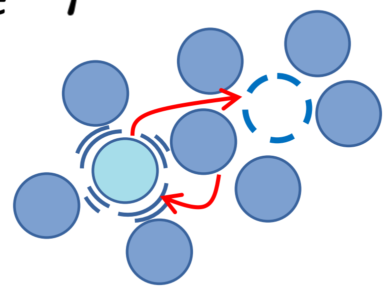
Continuum Liquid

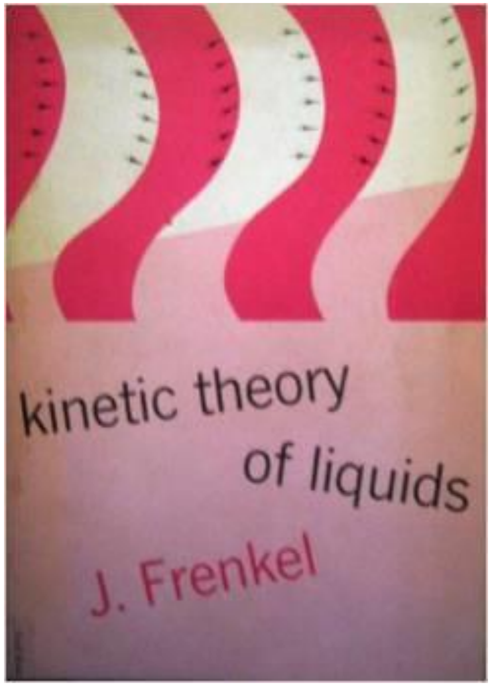
Continuum Solid

- **Flow** is the **Particle Rearrangement** process

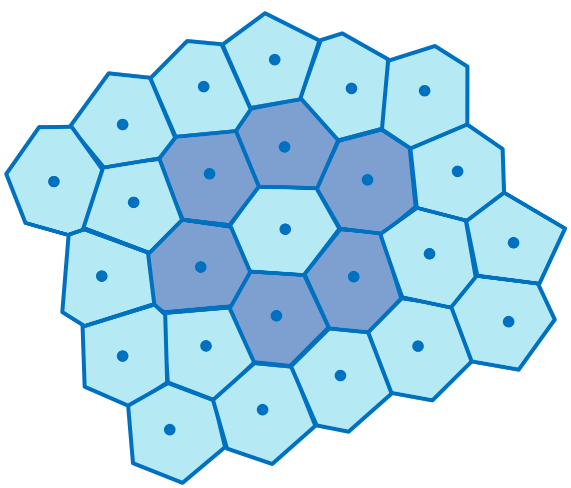
Particle rearrangements is a way to the Unified Flow Theory

- **Frenkel's idea** to describe **fluidity** of liquids is to introduce time τ

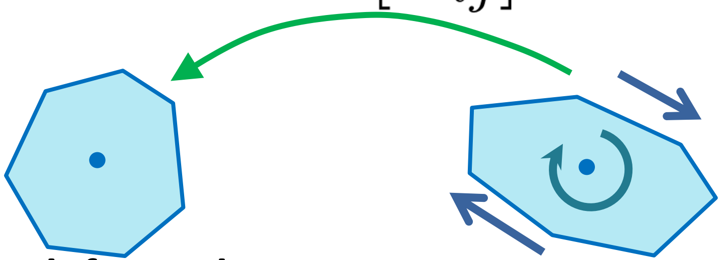




- Now, **molecules** = **fluid particles** or **fluid parcels**



$$\boldsymbol{A} = [A_{ij}]$$ Distortion (**non-symmetric**)



Undeformed particle

Deformed particle

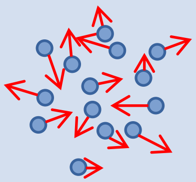
Main ingredients

- Dissipation **Time** $\mathcal{T}$
- **Distortion** field $\boldsymbol{A} = [A_{ij}]$
- **Energy potential** (equation of state):

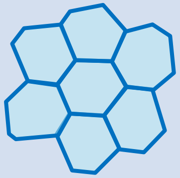
Equation of State

$$\mathcal{E}(\rho, s, \boldsymbol{A}, \boldsymbol{v}) = E_1(\rho, s) + E_2(\boldsymbol{A}) + E_3(\boldsymbol{v})$$

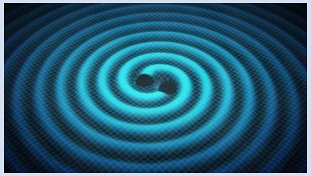
micro



meso



macro



Main ingredients

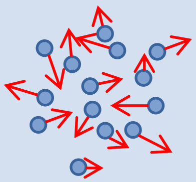
- Dissipation **Time** $\mathcal{T}$
- **Distortion** field $\boldsymbol{A} = [A_{ij}]$
- **Energy potential** (equation of state):

In classical theory

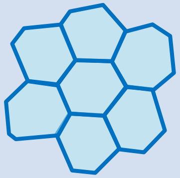
Equation of State

$$\mathcal{E}(\rho, s, \boldsymbol{A}, \boldsymbol{v}) = E_1(\rho, s) + E_2(\boldsymbol{A}) + E_3(\boldsymbol{v})$$

micro



meso



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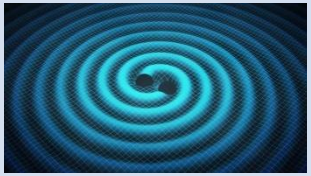


Governing equations

Momentum:

Visc. stresses

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial(\rho v_i v_k + \rho^2 \mathcal{E}_\rho \delta_{ik} + \rho A_{mi} \mathcal{E}_{A_{mk}})}{\partial x_k} = 0$$

Equation for the distortion:

$$\frac{\partial A_{ik}}{\partial t} + \frac{\partial A_{im} v_m}{\partial x_k} = -v_j \left(\frac{\partial A_{ik}}{\partial x_j} - \frac{\partial A_{ij}}{\partial x_k} \right) - \frac{\mathcal{E}_{A_{ij}}}{\tau}$$

$$\mathcal{E}(\rho, s, \boldsymbol{A}, \boldsymbol{v}) = E_1(\rho, s) + E_2(\boldsymbol{A}) + E_3(\boldsymbol{v})$$

Governing equations

Momentum:

Visc. stresses

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial(\rho v_i v_k + \rho^2 \mathcal{E}_\rho \delta_{ik} + \rho A_{mi} \mathcal{E}_{A_{mk}})}{\partial x_k} = 0$$

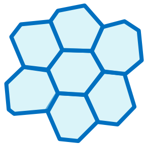
Navier-Stokes stress tensor:

$$\mu\left[\left(\frac{\partial v_i}{\partial x_k} + \frac{\partial v_i}{\partial x_k}\right) - \frac{2}{3}\frac{\partial v_m}{\partial x_m}\delta_{ik}\right]$$

$$\mathcal{E}(\rho, s, \boldsymbol{A}, \boldsymbol{v}) = E_1(\rho, s) + E_2(\boldsymbol{A}) + E_3(\boldsymbol{v})$$

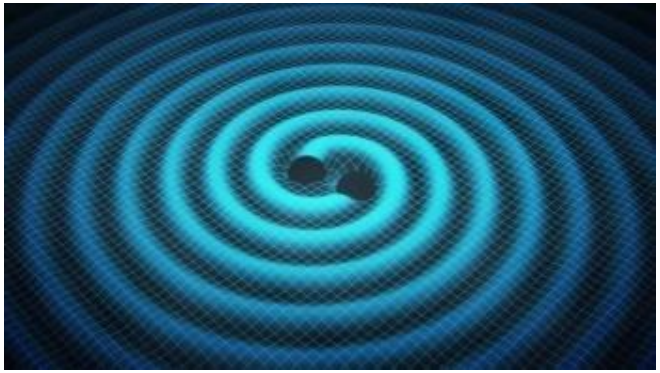
Wave theory

Fluid particles



Meso scale

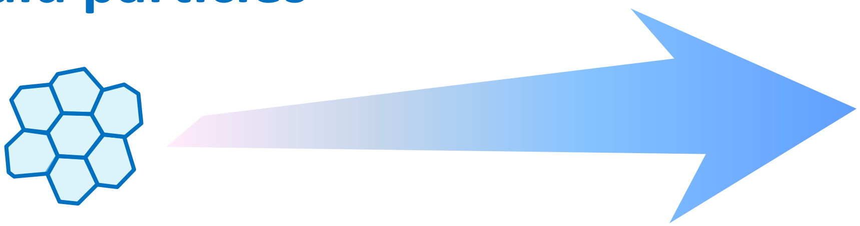
Waves



Macro scale

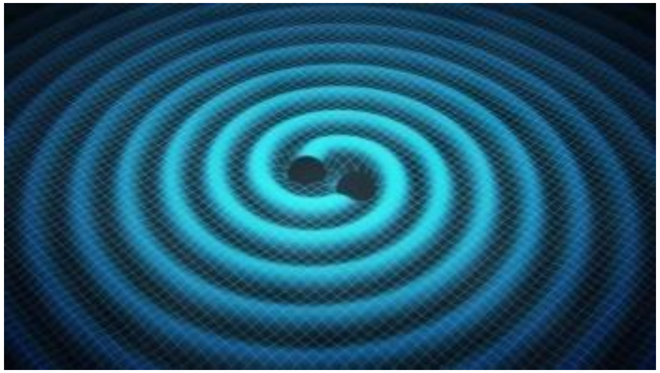
Wave theory

Fluid particles

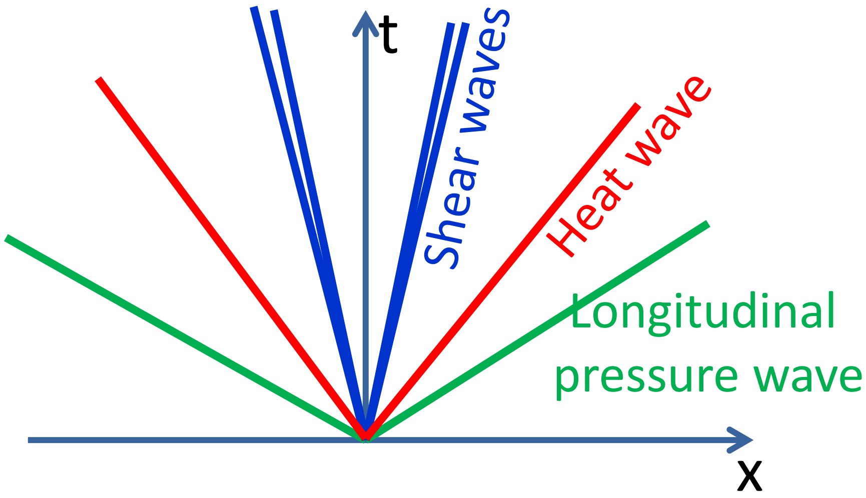


Meso scale

Waves

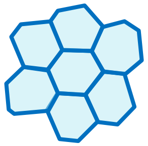


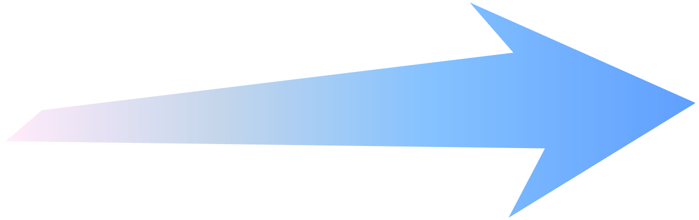
Macro scale



Wave theory

Fluid particles





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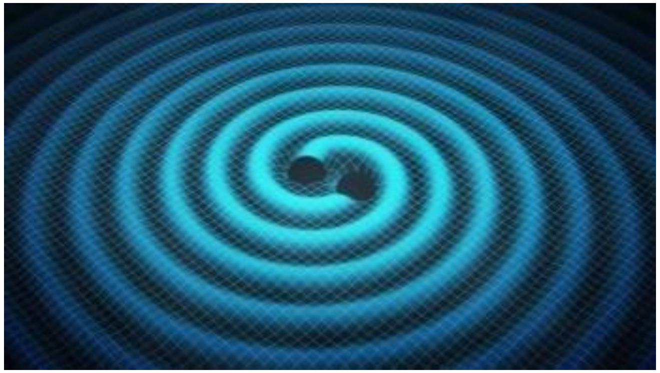
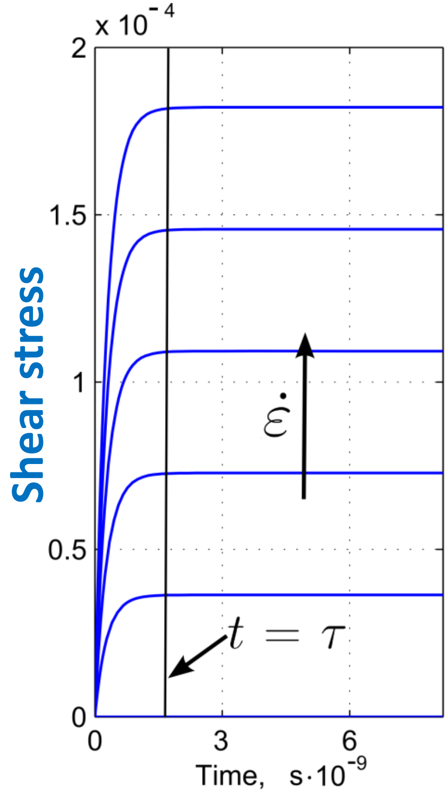
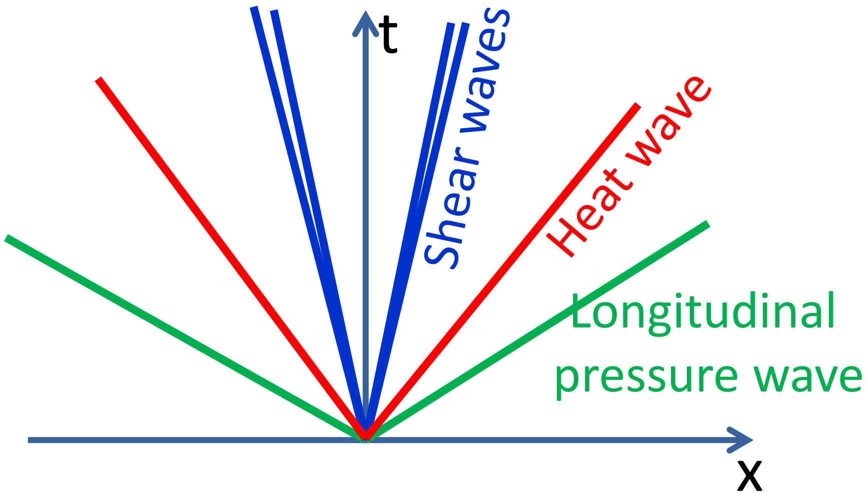


Meso scale

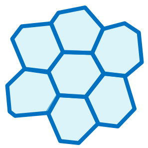
Macro scale





Wave theory

Fluid particles



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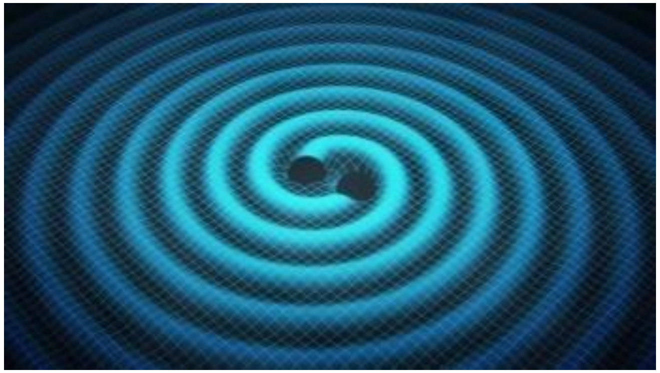
Waves



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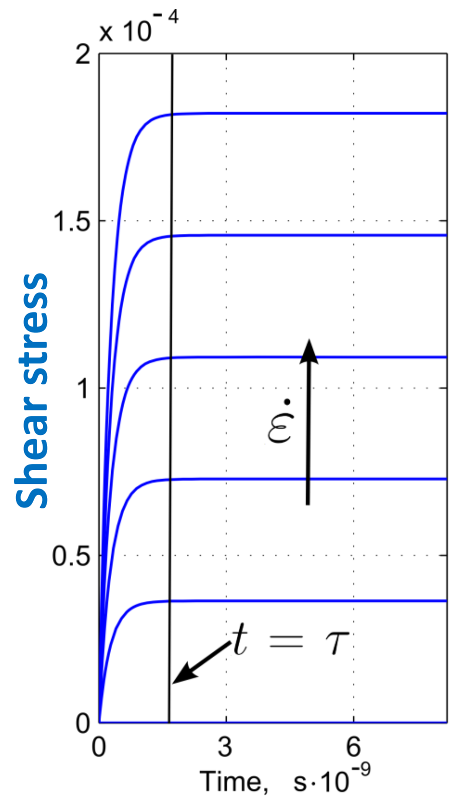
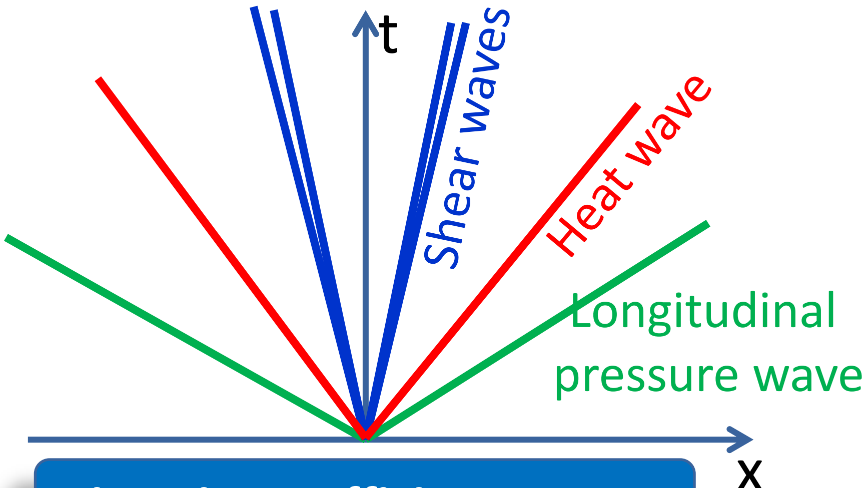




Viscosity coefficient

$$\eta = \varrho \tau c_t^2$$

Hyperbolic Heat Conduction

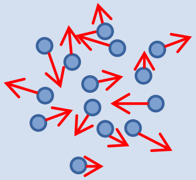
$$\frac{\partial \rho J_i}{\partial t} + \frac{\partial \left(\rho J_i v_k + E_s \delta_{ik}\right)}{\partial x_k} = -\frac{\rho E_{J_i}}{\theta}$$

$$\frac{\partial \rho s}{\partial t} + \frac{\partial \left(\rho s v_k + E_{J_k}\right)}{\partial x_k} = \frac{\rho}{\theta E_s} E_{J_i} E_{J_i} \geq 0$$

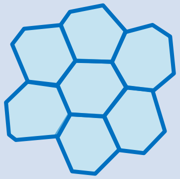
Equation of State

$$E(\rho, s, \boldsymbol{A}, \boldsymbol{J}, \boldsymbol{v}) = E_1(\rho, s) + E_2(\boldsymbol{A}, \boldsymbol{J}) + E_3(\boldsymbol{v})$$

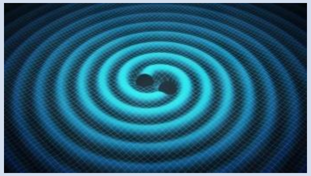
micro



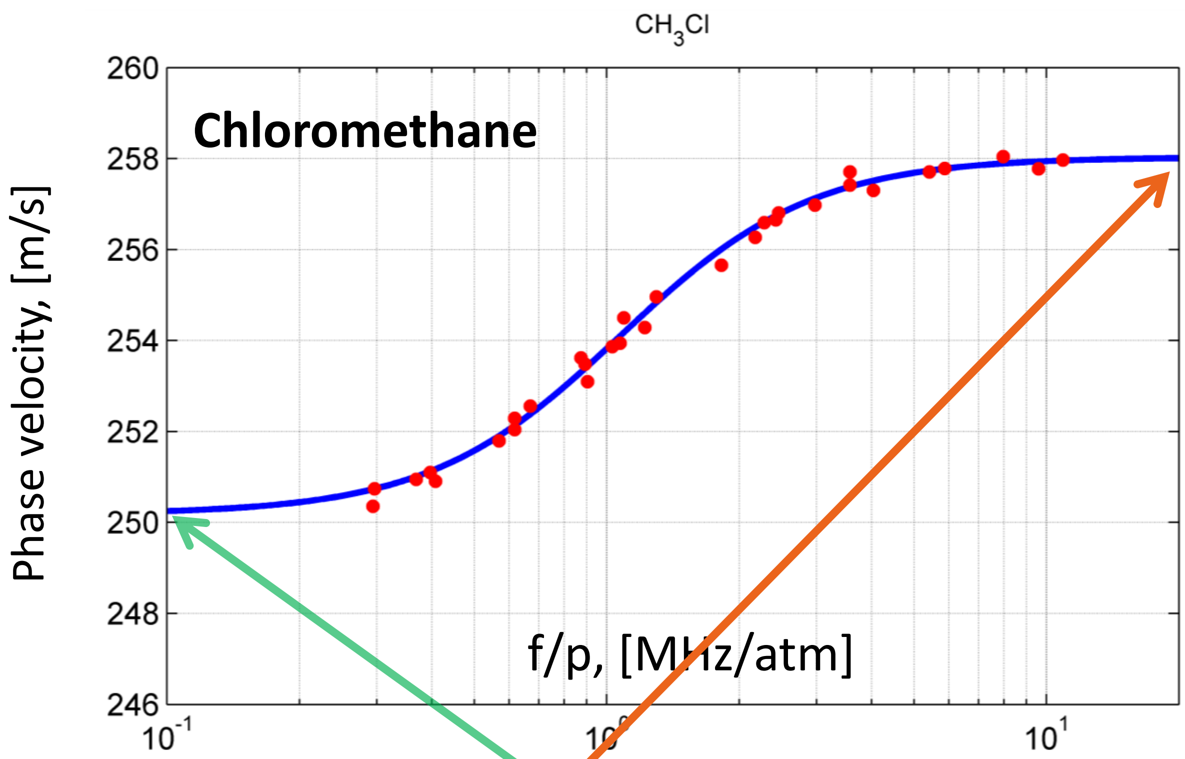
meso



macro



But how to get the parameters? High frequency measurements



$$c_\infty = \sqrt{c_0^2 + \frac{4}{3}c_t^2} \longrightarrow c_t \approx 50 \text{ [m/s]}$$

Viscosity coefficient

$$\eta = \varrho \tau c_t^2 \longrightarrow \tau \approx 10^{-8} [\text{sec}]$$

Ref: Data from **Sette, Busala, Hubbard,** *The Journal of Chem. Phys.*, ***23*** *(5), 1955*

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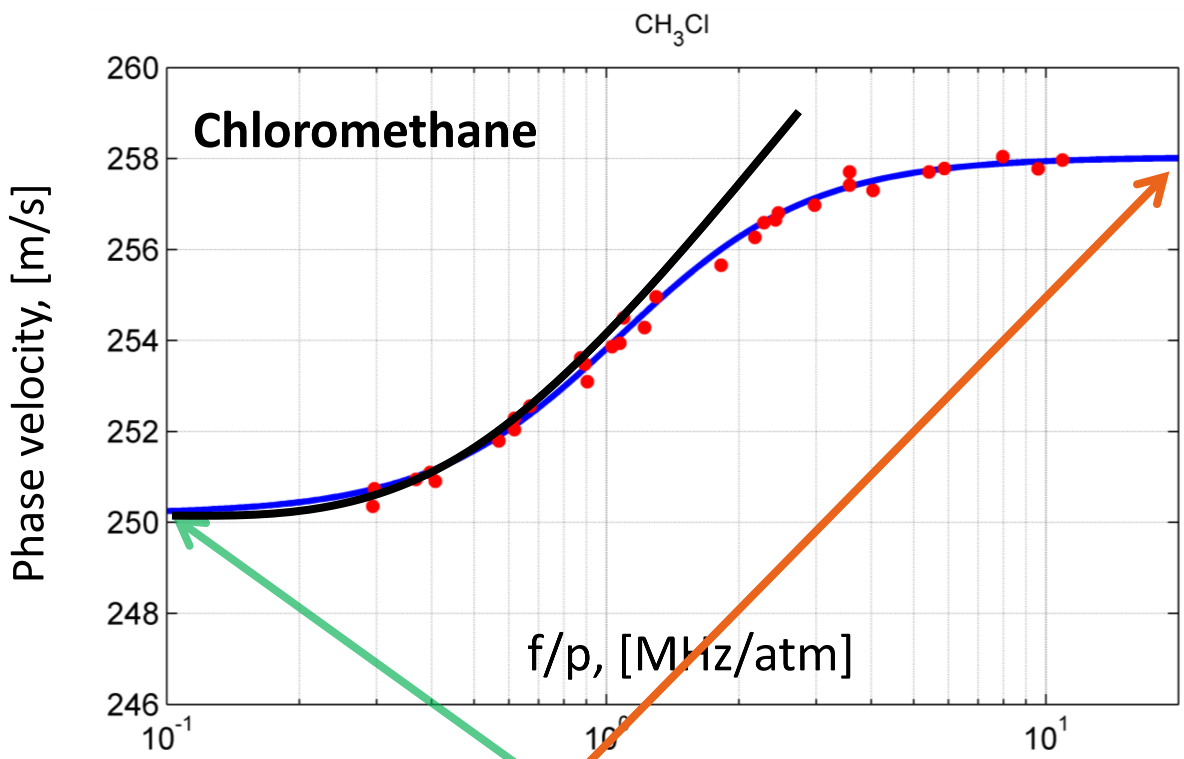

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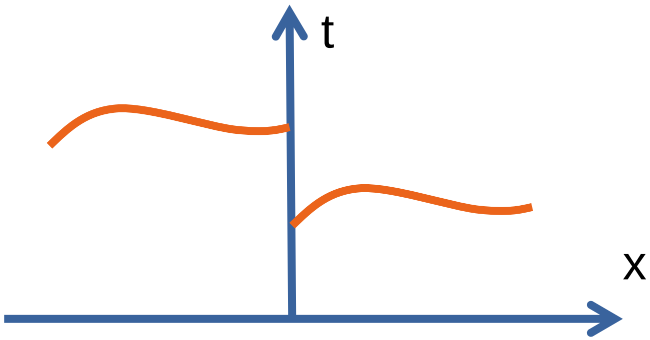
ADER-WENO-FVM-DG framework, (also $P_N P_M$ methods)

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{q})}{\partial x} = \boldsymbol{S}(\boldsymbol{q})$$

$$\boldsymbol{q}_i^{n+1} = \boldsymbol{q}_i^n - \frac{\Delta t}{\Delta x_i}\left(\boldsymbol{F}_{i+1/2} - \boldsymbol{F}_{i-1/2}\right) + \Delta t \boldsymbol{S}_i$$



Generalized Riemann Problem
GRP
(smoothed initial data)

1. **WENO reconstruction (**degree *N***)**
2. **Solve GRP coupled with the source terms (**degree *M*>*N***)**
   (Cauchy-Kovalevski or DG**)**
3. **Update at n+1**

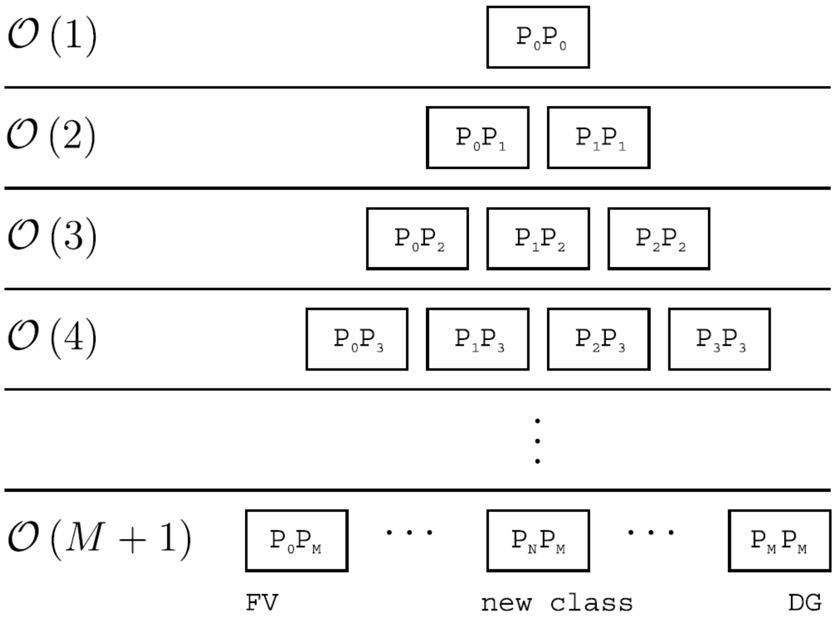
See papers by E. Toro, V. Titarev, M. Dumbser since 2000

ADER-WENO-FVM-DG framework, (also $P_N P_M$ methods)

$$\frac{\partial \boldsymbol{q}}{\partial t} + \frac{\partial \boldsymbol{F}(\boldsymbol{q})}{\partial x} = \boldsymbol{S}(\boldsymbol{q})$$

$$\boldsymbol{q}_i^{n+1} = \boldsymbol{q}_i^{n} - \frac{\Delta t}{\Delta x_i}\left(\boldsymbol{F}_{i+1/2} - \boldsymbol{F}_{i-1/2}\right) + \Delta$$

Unified $P_N P_M$ family of methods

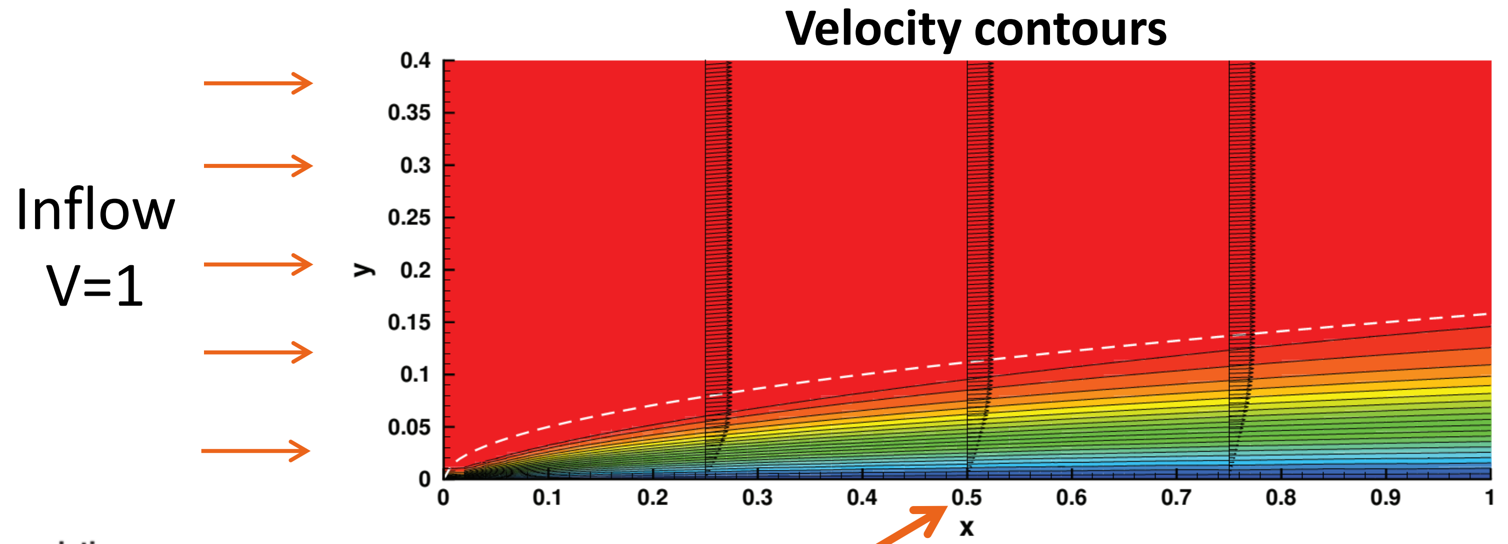


See papers by Michael Dumbser since ~2008

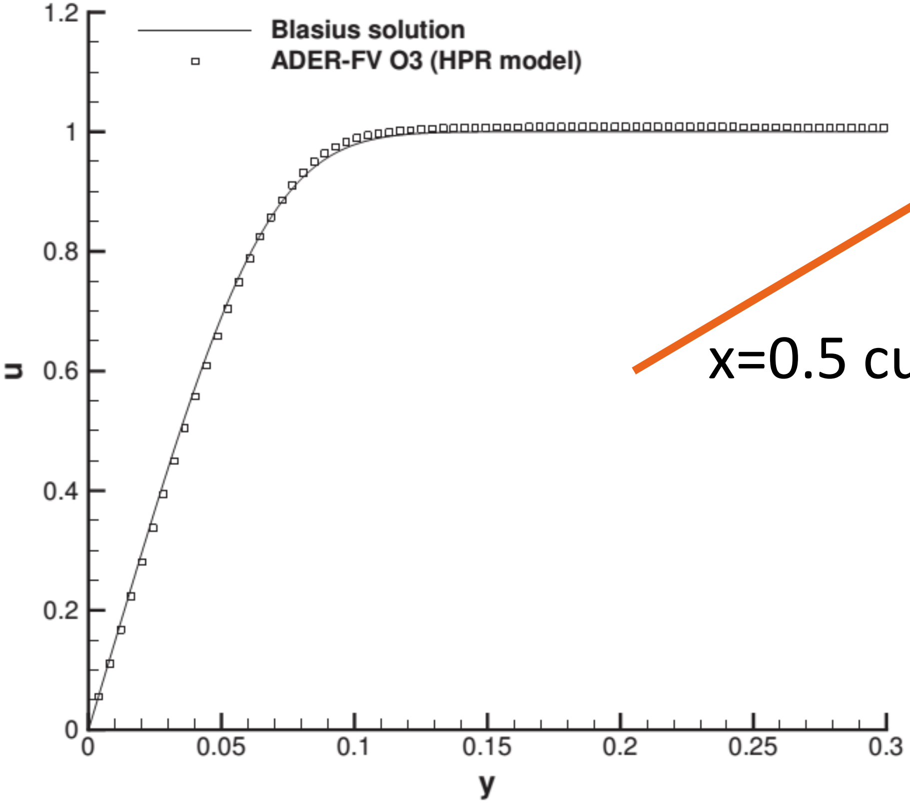
Code characteristics:

- Explicit globally (implicit locally)
- Massively Parallel
- Arbitrary order (up to 10 implemented)
- Equally High Order in both, **space and time**
- One step in time
- Robust WENO FV or ultra compact DG
- Unstructured grids (complex geometries)
- Stiff source terms (asymptotic preserving)

Blasius boundary layer, *Re*=1000

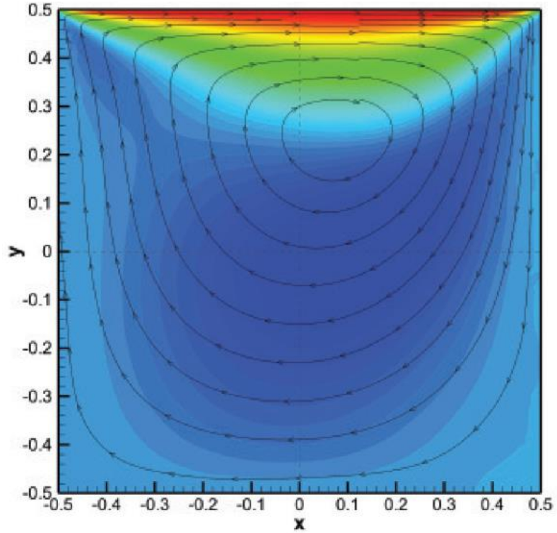


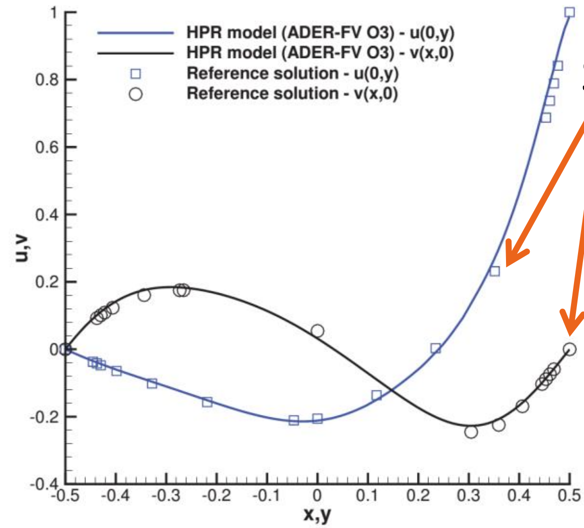
x=0.5 cut



Lid driven cavity flow at *Re*=100

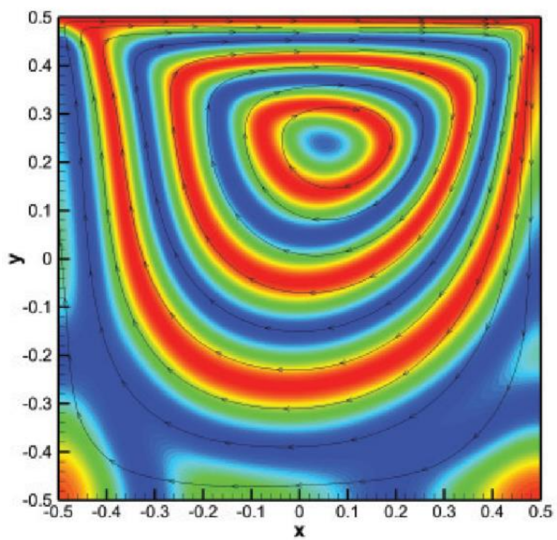
Velocity, u

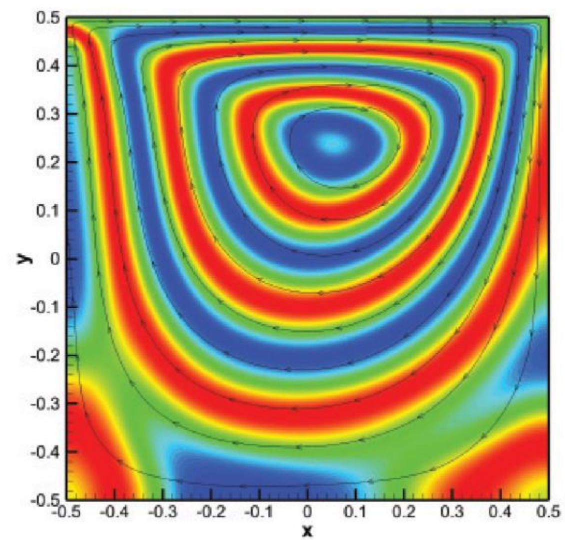




Symbols are NS model, velocities

A_{11}





A_{12}

Double shear layer, visc=$2\cdot10^{-4}$

Vorticity

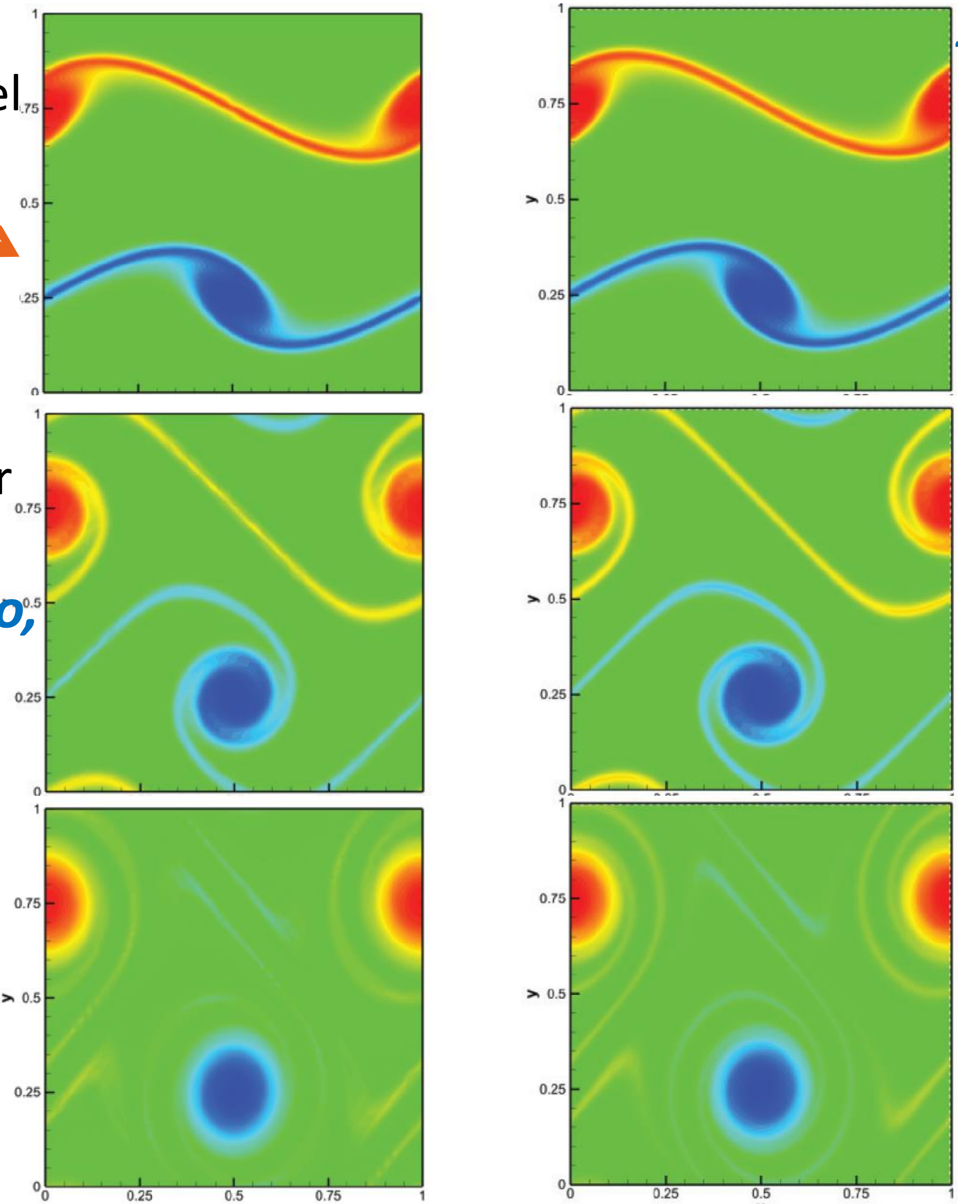
Left: Hyperbolic model

ADER-WENO 4th order scheme from

Dumbser, Enaux, Toro, 2008

Right: Navier-Stokes model staggered Semi-implicit DG P3

Tavelli , Dumbser 2014



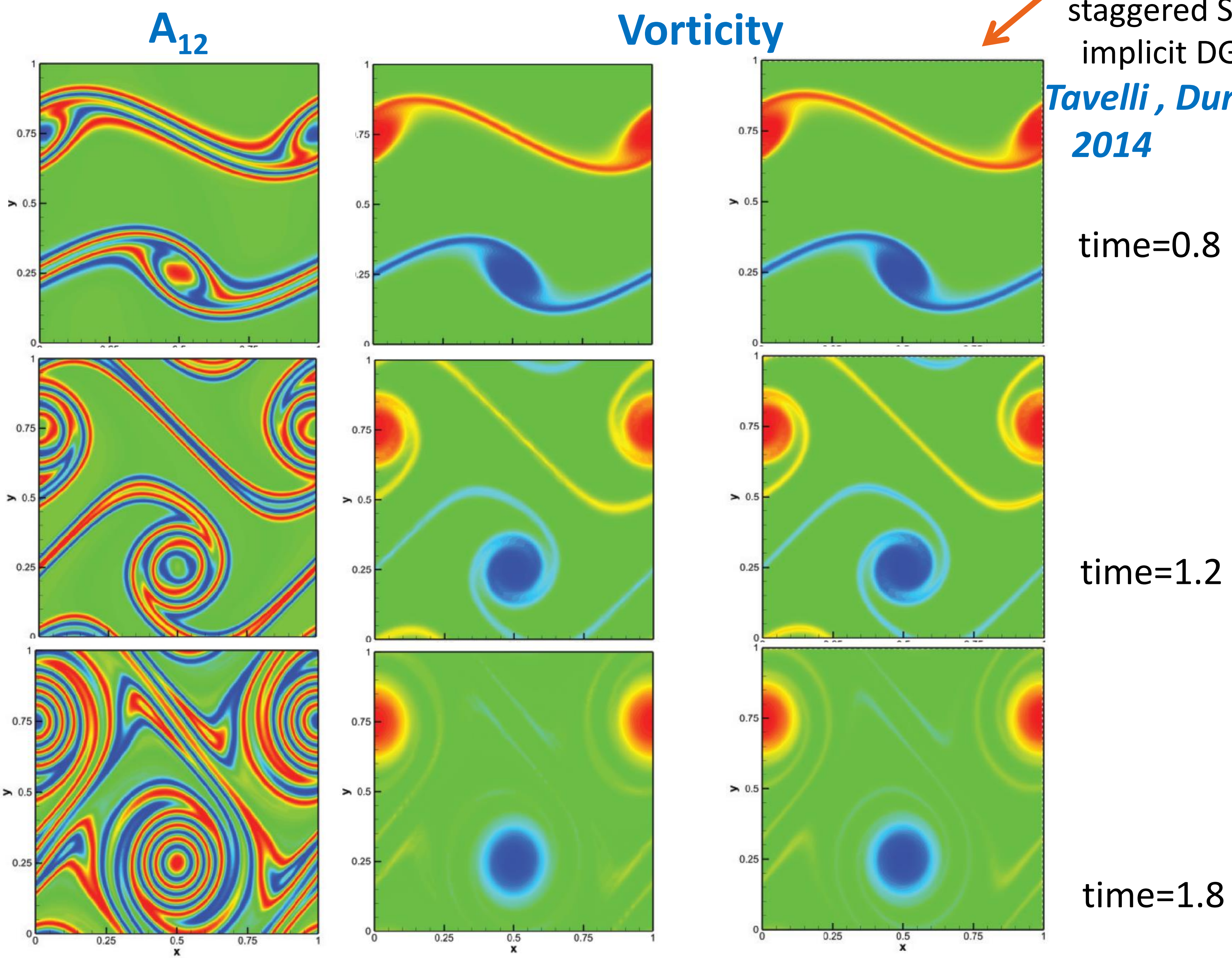
time=0.8

time=1.2

time=1.8

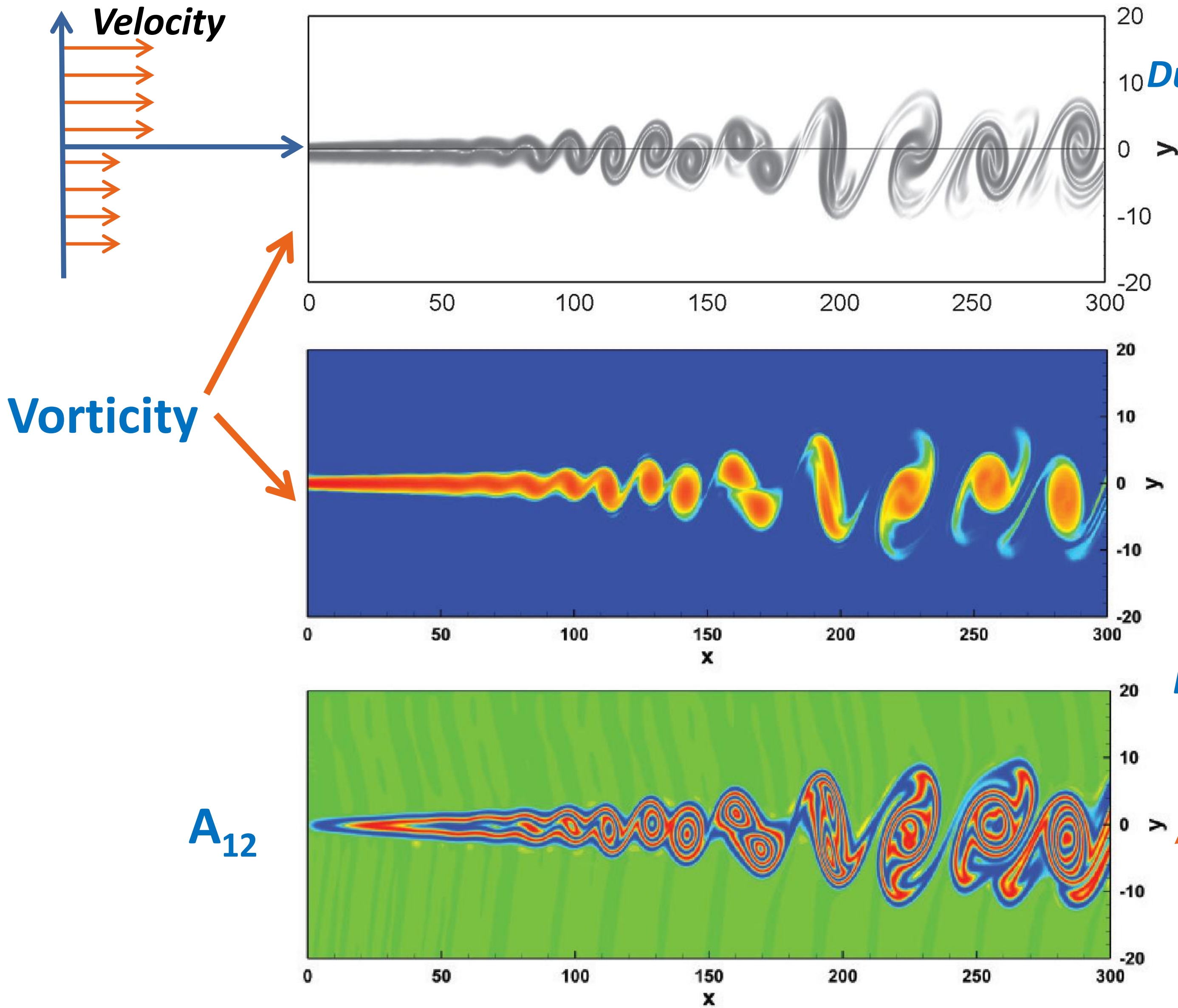
Double shear layer,

***Right**: Navier-Stokes model staggered Semi-implicit DG P3*
Tavelli , Dumbser 2014



Compressible mixing layer, *Re*=250

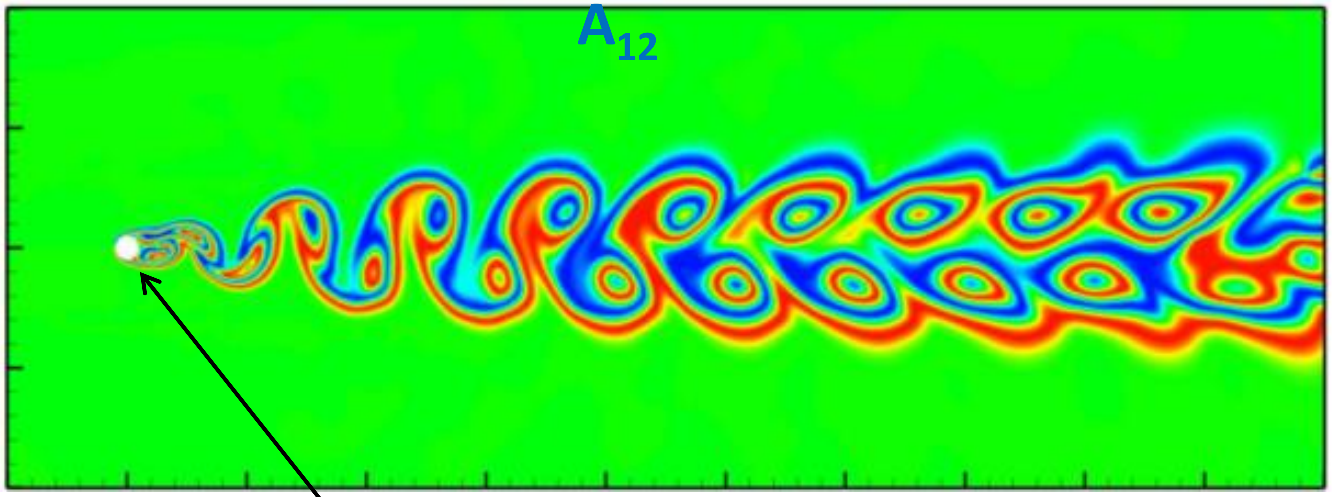
Top: 6^{th} order P_NP_M scheme
Navier-Stokes model
Dumbser, Zanotti, 2009



Hyperbolic model
3^{rd} order ADER-WENO
Dumbser, Enaux, Toro, 2008

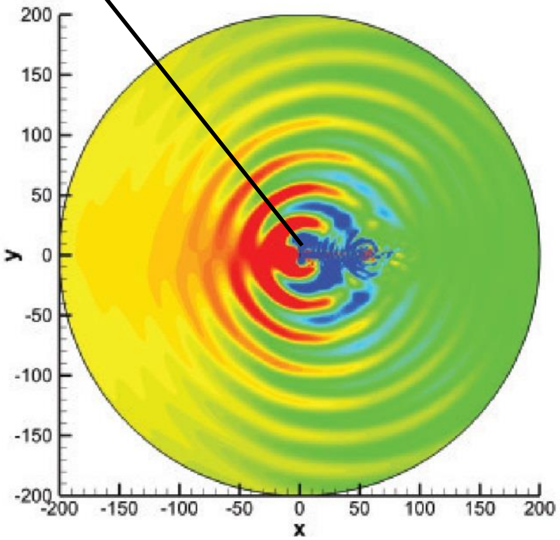
Flow around a circular cylinder, *Re*=150

Flow direction



Strouhal number

$$\mathrm{St} = \frac{fL}{U} = 0.18$$



Pressure field.

Full computational domain

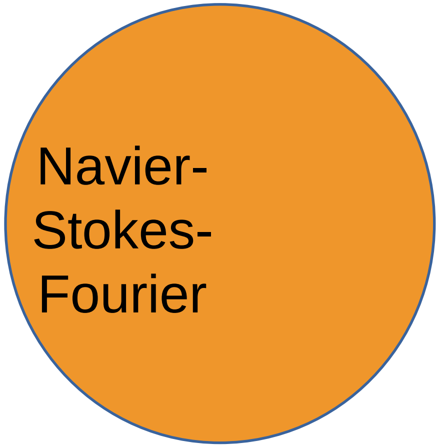
Why would one use order Hyperbolic PDEs?

Severe **time step restriction in Parabolic problems** (explicit scheme) **critical** for complex flows and HPC
(# *turbulence, viscoacoustics, 2-phase pore-scale modeling, etc.*)

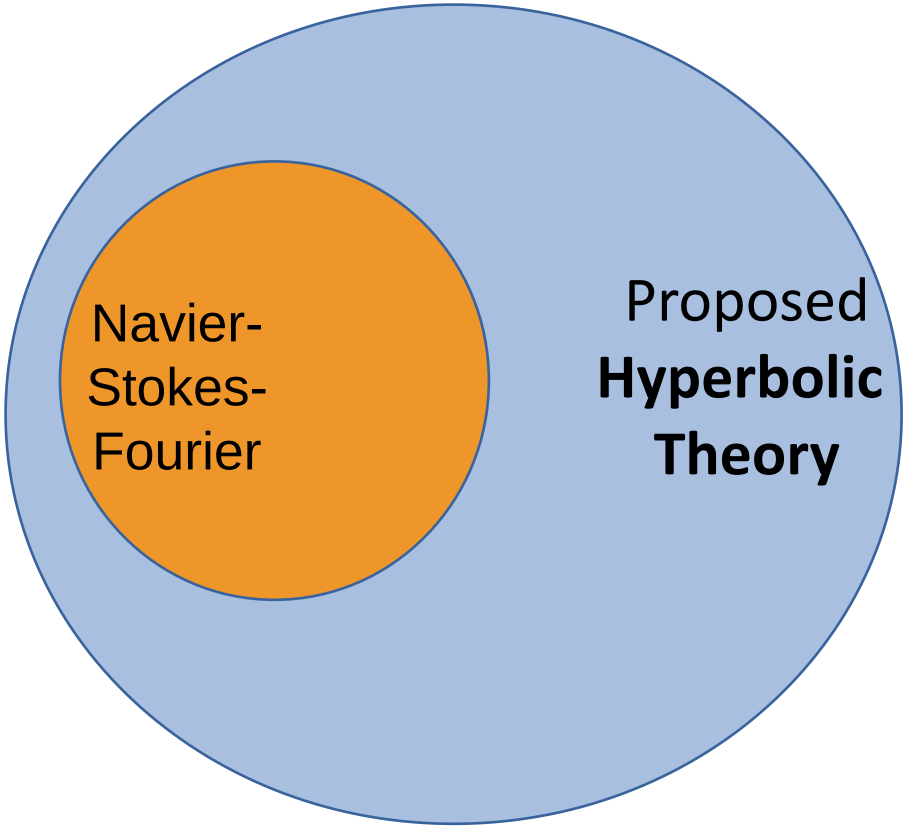
	2nd order Parabolic		**1st order Hyperbolic**	
	Navier-Stokes equations		**Extended HPR model**	
Mesh	time steps	CPU time	time steps	CPU time
ADER finite volume scheme ($\mathcal{O}3$)				
100	1587	18.7	479	98.0
200	5535	112.2	926	298.3
ADER-DG scheme (P3)				
100	87080	2317.2	4545	1743
200	340646	18476	9059	6133

$$\Delta t \sim (\Delta x)^2 \qquad \Delta t \sim \Delta x$$

Turbulence



Turbulence



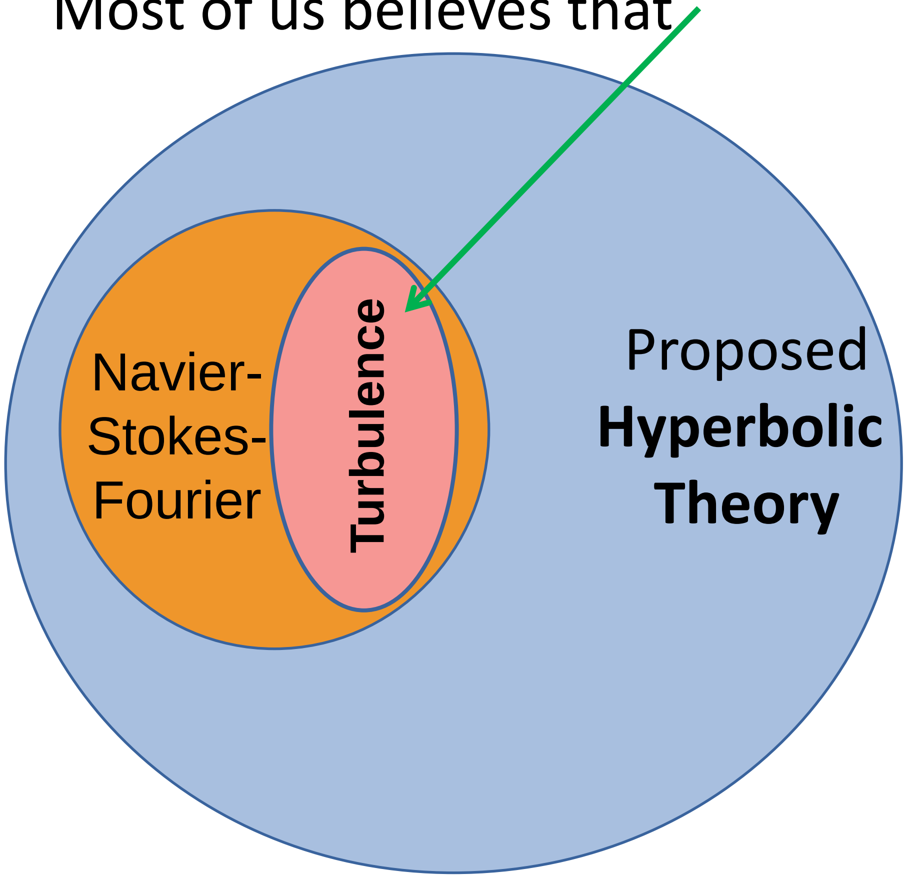
Now we have 2 **fundamentally different** models

Parabolic vs. Hyperbolic

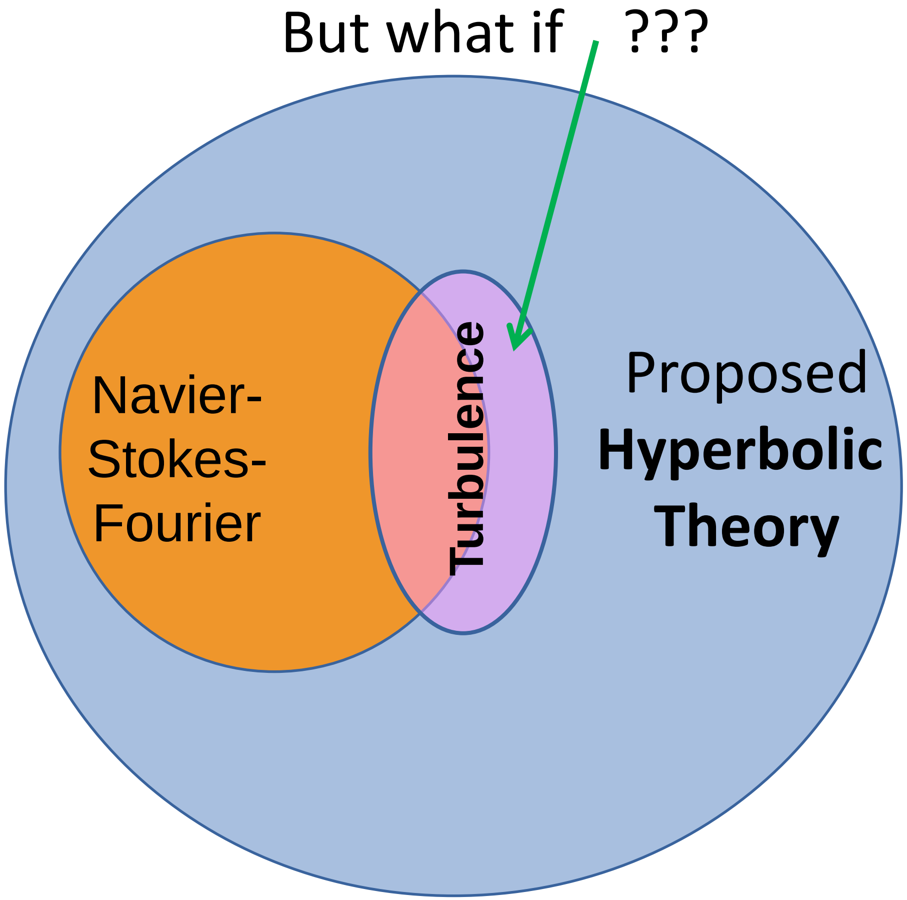
Dumbser, Peshkov, Romenski, Zanotti
"High order ADER schemes for a unified first order hyperbolic formulation of continuum mechanics: viscous heat-conducting fluids and elastic solids"
Journal of Computational Physics. 2016. (Open access)

Turbulence

Most of us believes that

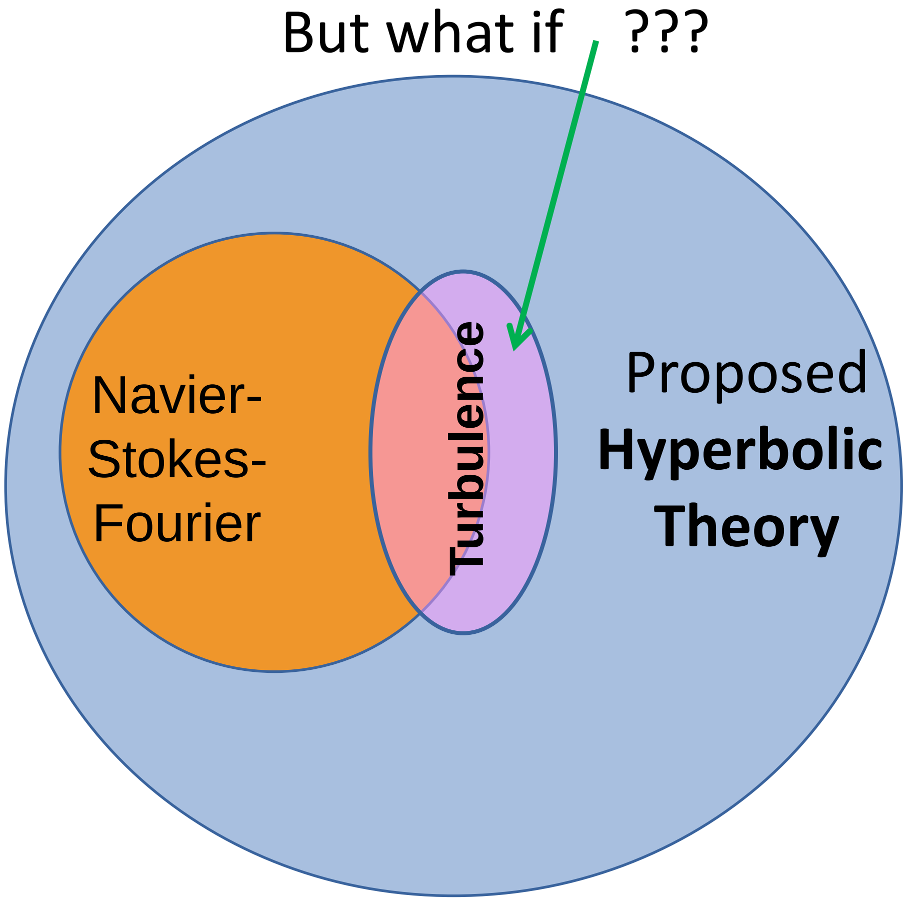


Turbulence



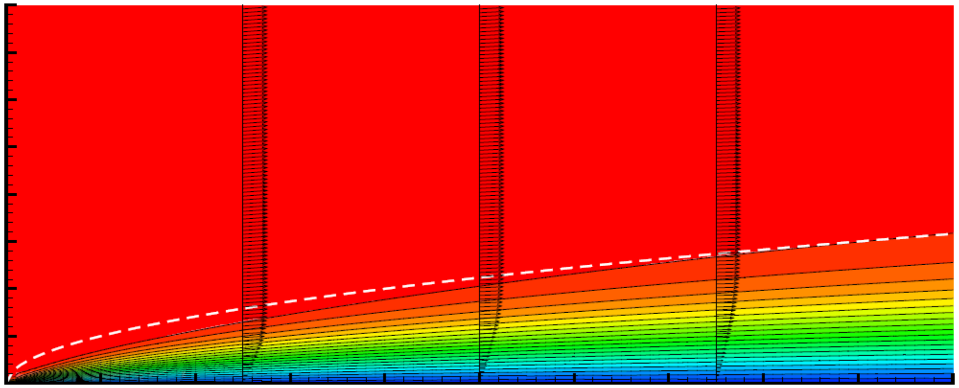
But what if ???
Turbulence
Navier-Stokes-Fourier
Proposed Hyperbolic Theory

Turbulence

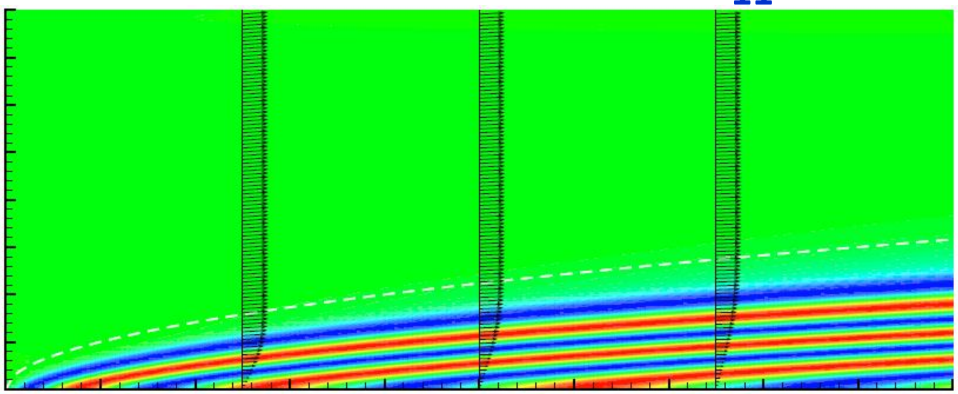


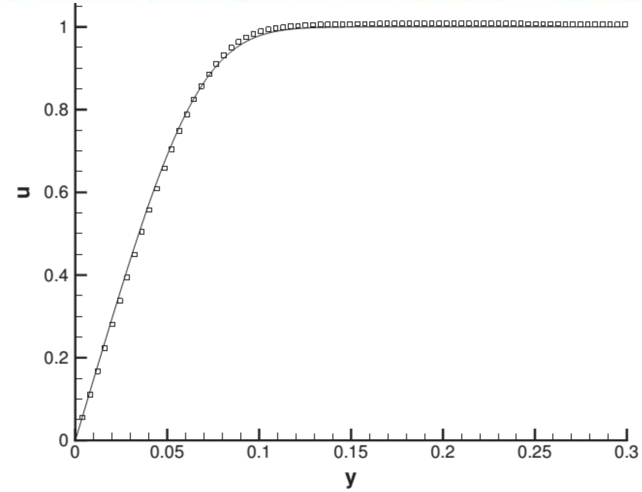
Blasius boundary layer problem

Velocity

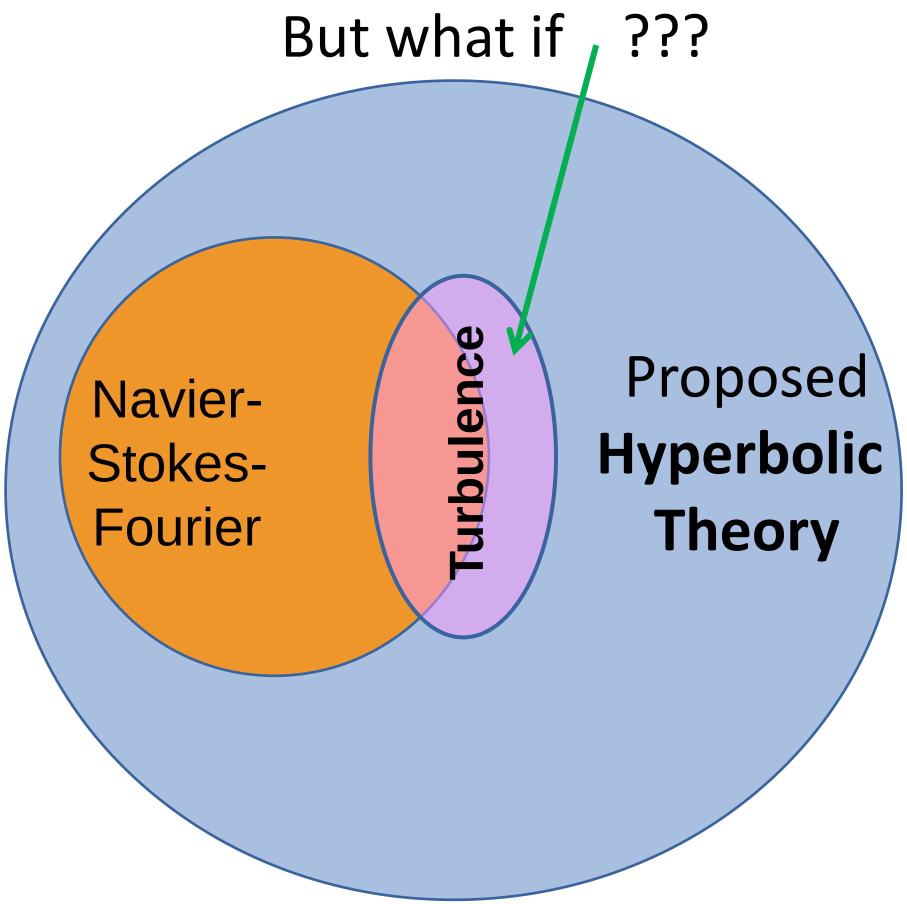


Distortion, A_{11}

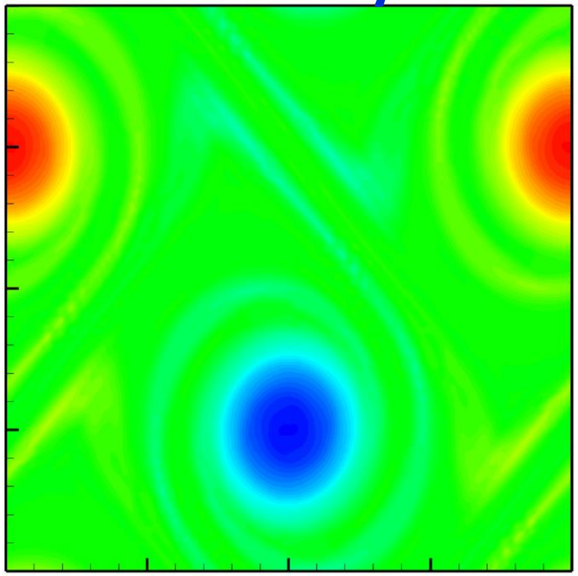




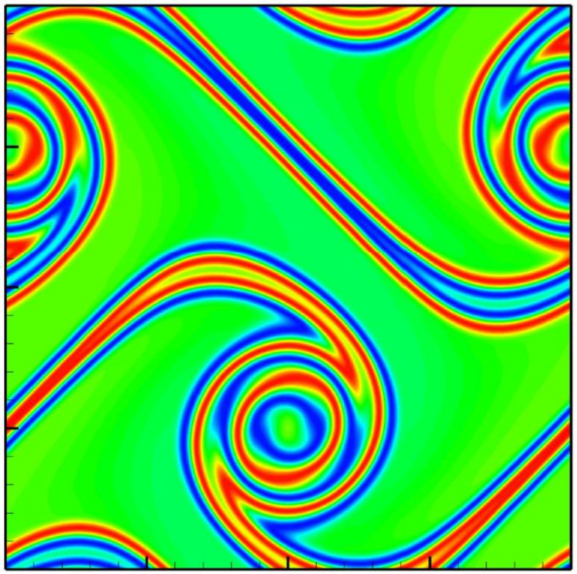
Turbulence



Vorticity

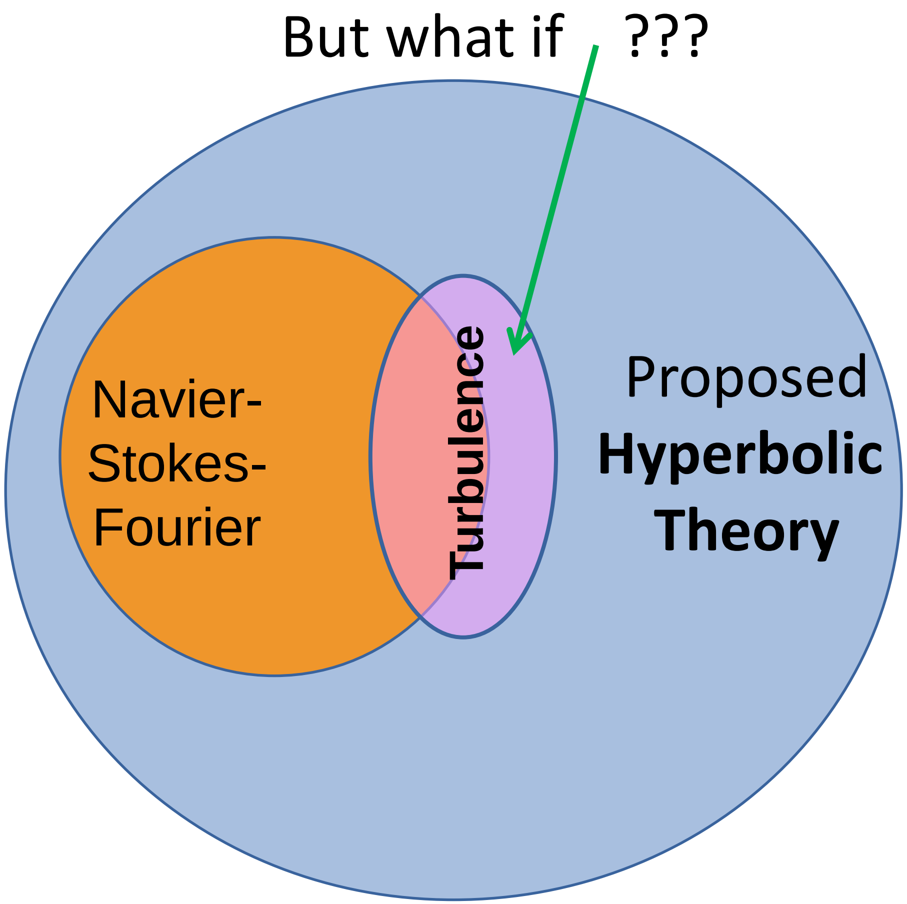


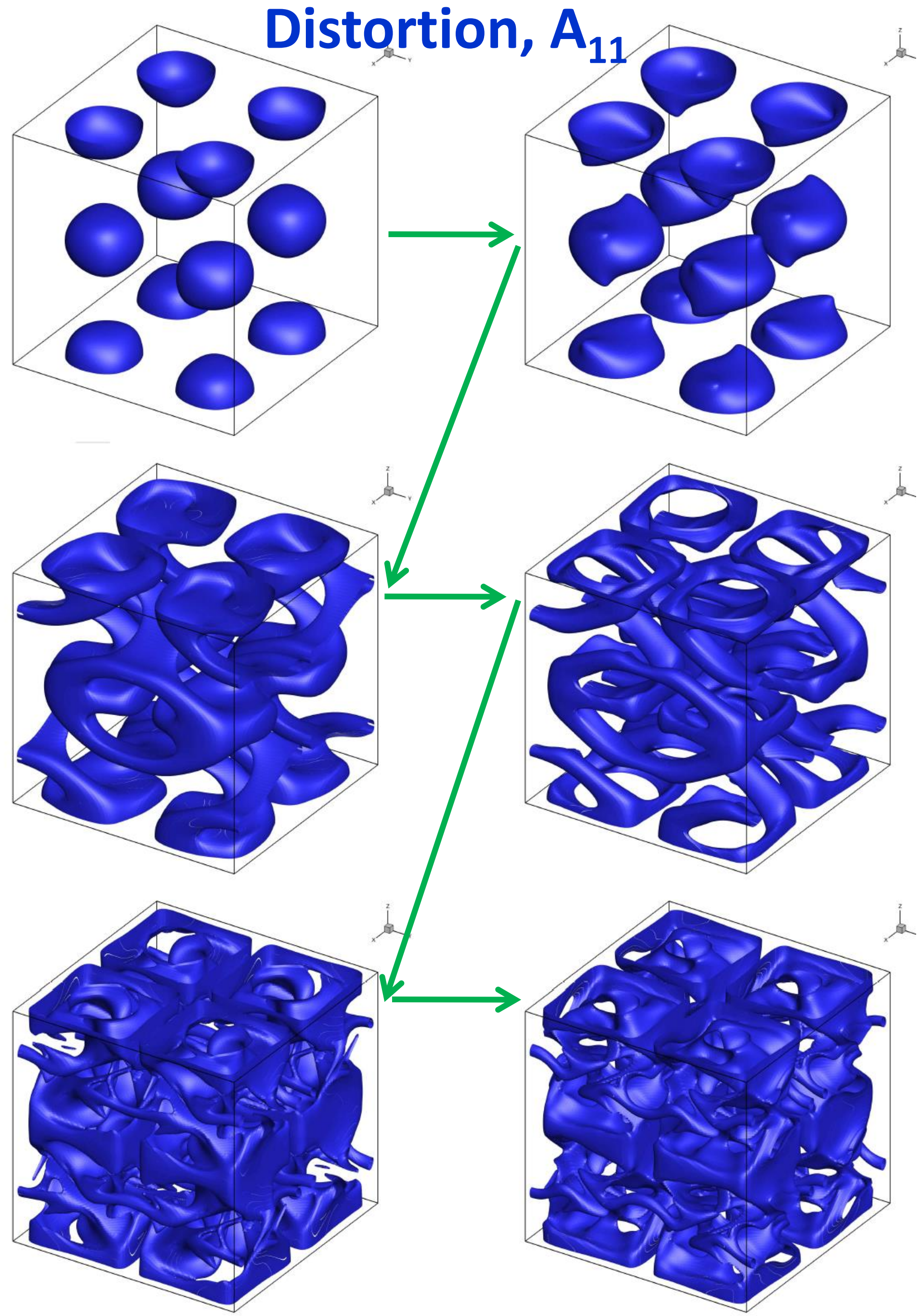
Distortion, A_{11}



Double shear layer problem

Turbulence

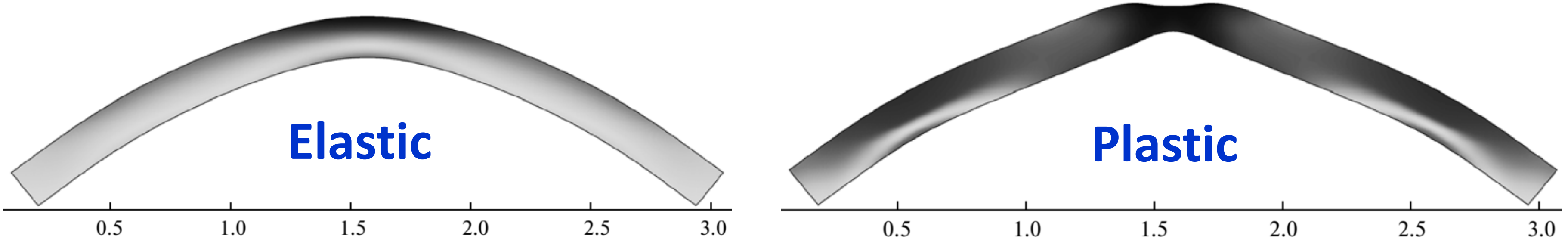




3D Taylor-Green vortex

Solid dynamics

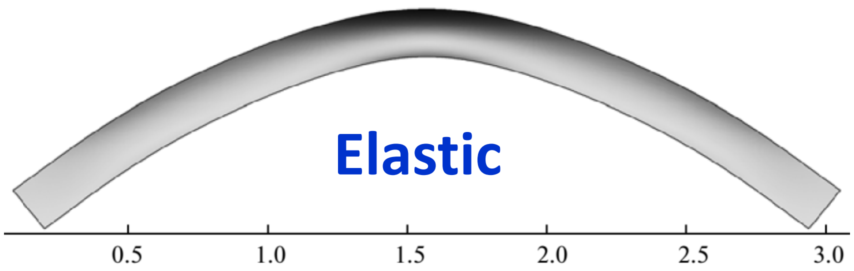
Using the **same(!) system of PDEs** we can simulate **dynamics of solids** as well

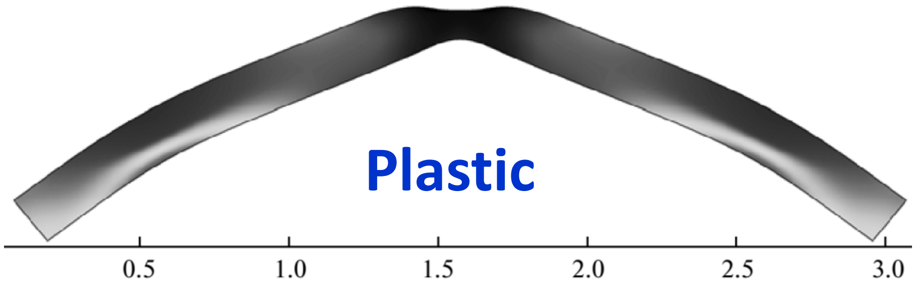


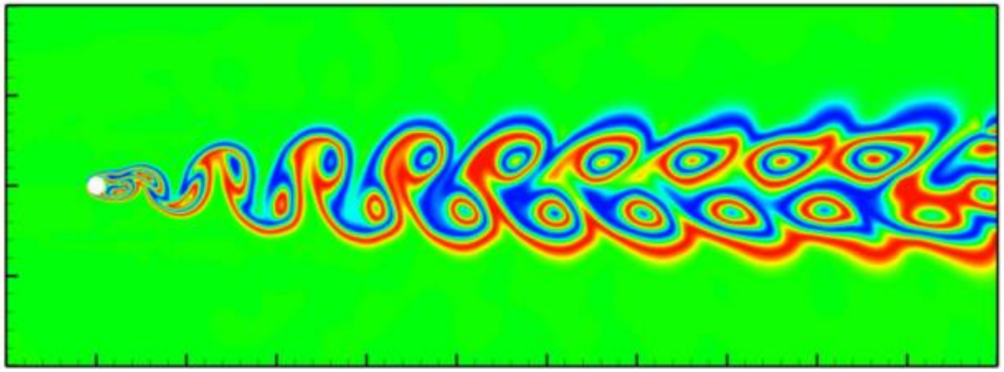
Bending of a plate

Solid dynamics

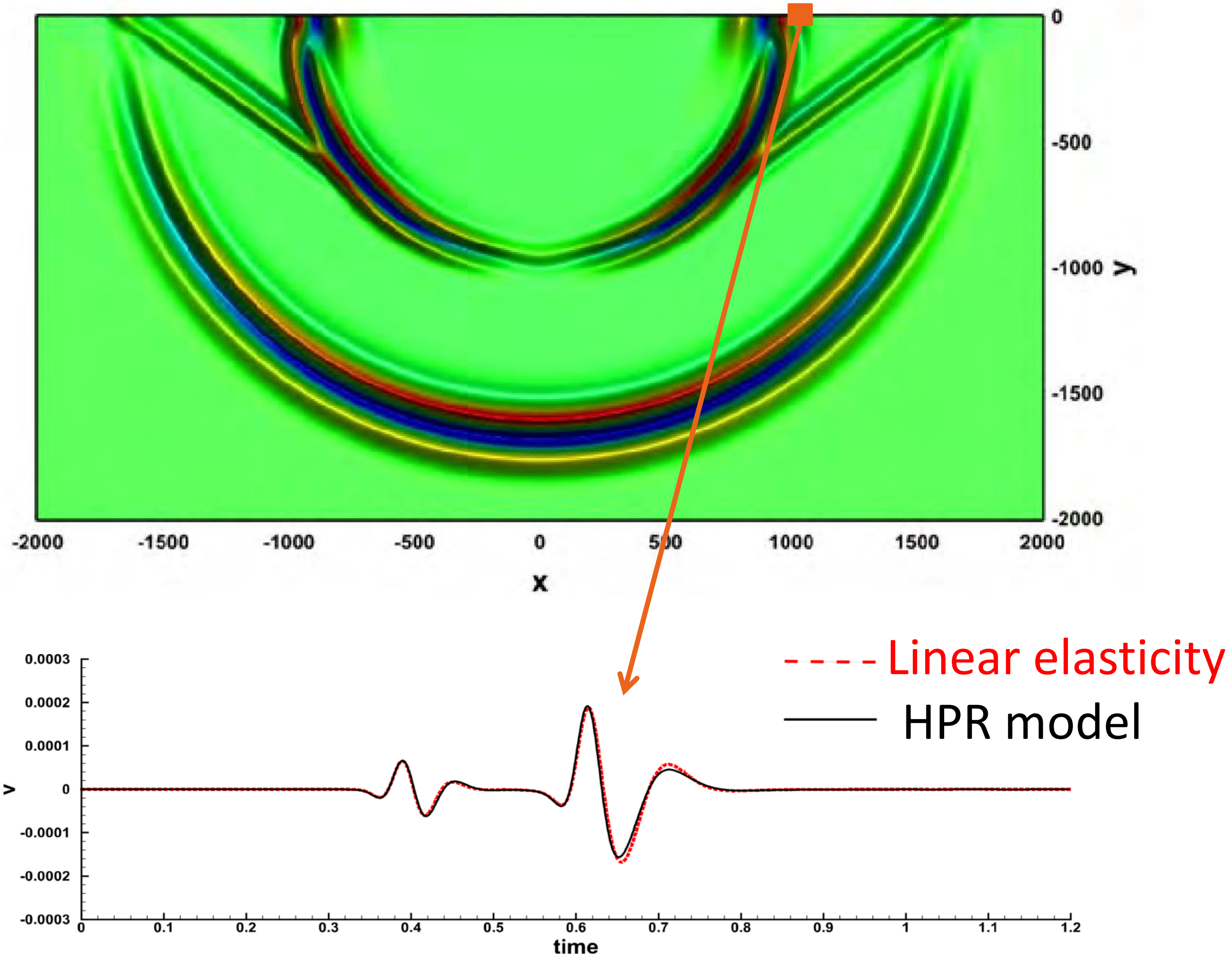
Using the **same(!) system of PDEs** we can simulate **dynamics of solids** as well







Seismic wave propagation



Poroelasticity

Biot's Theory

$$\rho_{11}\ddot{\boldsymbol{U}} + \rho_{12}\ddot{\boldsymbol{V}} - (P - N)\nabla \mathrm{div}\boldsymbol{U} - Q\nabla \mathrm{div}\boldsymbol{V} - N\Delta\boldsymbol{U} + b(\dot{\boldsymbol{U}} - \dot{\boldsymbol{V}}) = 0$$

$$\rho_{22}\ddot{\boldsymbol{V}} + \rho_{12}\ddot{\boldsymbol{U}} - Q\nabla \mathrm{div}\boldsymbol{U} - R\nabla \mathrm{div}\boldsymbol{V} + b(\dot{\boldsymbol{V}} - \dot{\boldsymbol{U}}) = 0$$

Drawbacks:

- Established as a **Linear theory** from the very beginning
  - modification problems (viscoelastic media, fraction time derivative, etc.)
- Composite elastic modulus ***Q*** of the whole media (phase coupling parameter)
  - measurement problems
  - interpretation

Nonlinear Mixture Theory: state parameters

$\boldsymbol{v}_s, \ \boldsymbol{v}_f$ Velocities of the solid and fluid phase

$\boldsymbol{F} = \boldsymbol{A}^{-1}$ Deformation gradient

α_s Volume fraction of the solid matrix

$\rho = \alpha_s \rho_s + \alpha_f \rho_f$ Mixture density

The missing parameter in the Biot's theory

$$c_s = \frac{\alpha_s \rho_s}{\rho}$$

Mass fractions (concentrations)

Nonlinear Mixture Theory: state parameters

$$v_s,\ v_f \Rightarrow$$

$$v = c_s v_s + c_f v_f$$

$$w = v_s - v_f$$

Solid-Fluid mixture model

$$\frac{\partial \rho v_i}{\partial t} + \frac{(\rho v_i v_k + \rho^2 E_\rho \delta_{ik} + \rho w_i E_{w_k} - \rho F_{km} E_{F_{im}})}{\partial x_k} = 0$$ **momentum**

$$\frac{\partial F_{ij}}{\partial t} + \frac{(\rho F_{ij} v_k - \rho F_{kj} v_i)}{\partial x_k} = 0$$ **deformation**

$$\frac{\partial \rho c_s}{\partial t} + \frac{(\rho c_s v_k + \rho E_{w_k})}{\partial x_k} = 0$$ **Mass fraction**

$$\frac{\partial w_k}{\partial t} + \frac{(v_m w_m + E_{c_s})}{\partial x_k} = e_{klj}\omega_j - \chi E_{w_k}$$ **Relative velocity**

$$\frac{\partial \rho \alpha_s}{\partial t} + \frac{\rho \alpha_s v_k}{\partial x_k} = -\lambda \rho E_{\alpha_s}$$ **Volume fraction**

$$\frac{\partial \rho}{\partial t} + \frac{\rho v_k}{\partial x_k} = 0$$

Linearised model: single pressure model

$$\frac{\partial \boldsymbol{q}}{\partial t} + A(\boldsymbol{q}^0)\frac{\partial \boldsymbol{q}}{\partial x} = f \qquad \boldsymbol{q} = (\boldsymbol{v}_s, \boldsymbol{v}_f, p, \varepsilon_{ij})$$

$$f = \left(-\frac{\rho_s^0 c_f^0 (\boldsymbol{v}_s - \boldsymbol{v}_f)}{\tau}, -\frac{\rho_f^0 c_s^0 (\boldsymbol{v}_f - \boldsymbol{v}_s)}{\tau}, 0, 0_{ij} \right)$$

Linearised model: single pressure model

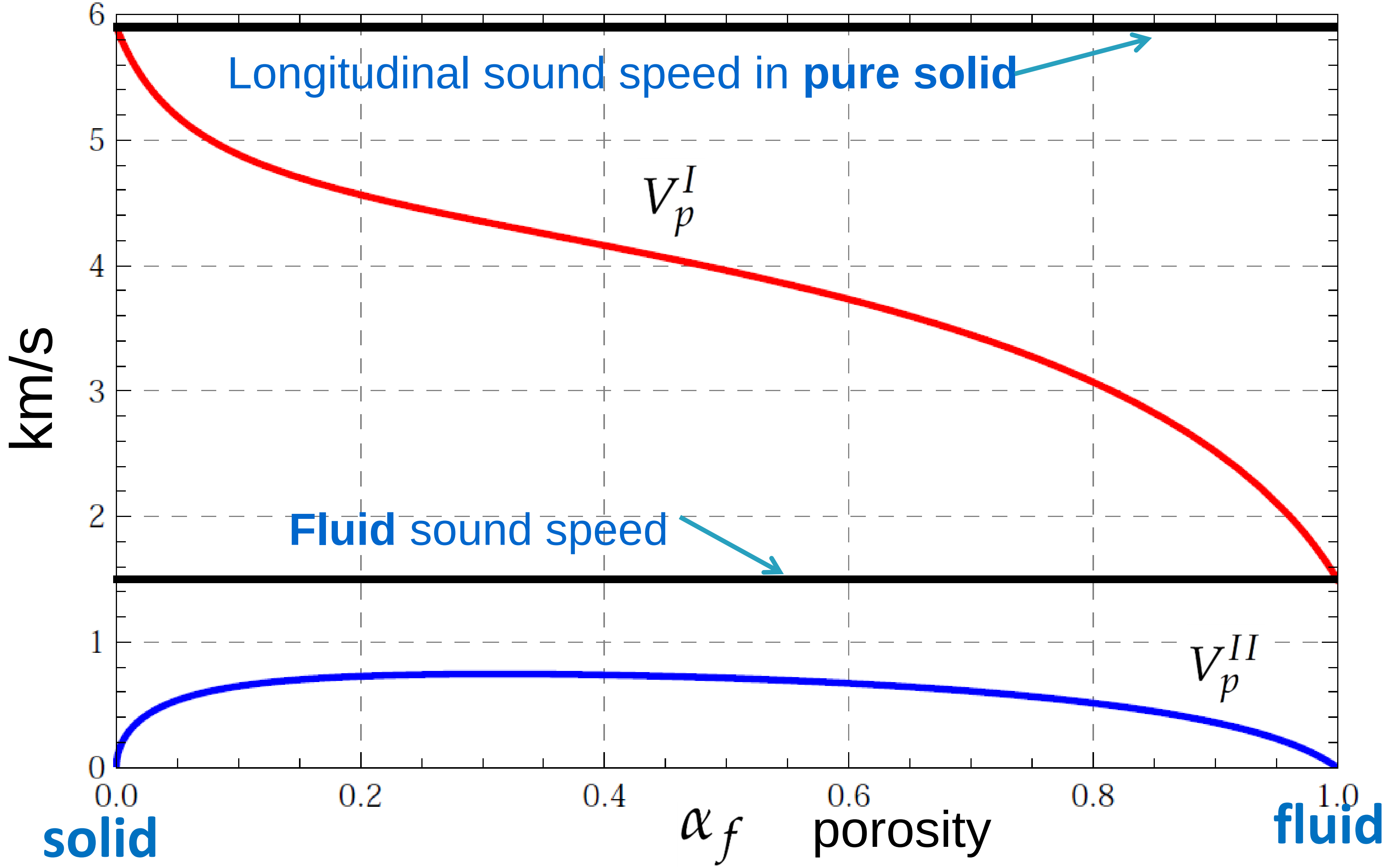
$$\frac{\partial \boldsymbol{q}}{\partial t} + A(\boldsymbol{q}^0)\frac{\partial \boldsymbol{q}}{\partial x} = f \qquad \boldsymbol{q} = (\boldsymbol{v}_s, \boldsymbol{v}_f, p, \varepsilon_{ij})$$

$$f = \left(-\frac{\rho_s^0 c_f^0 (\boldsymbol{v}_s - \boldsymbol{v}_f)}{\tau}, -\frac{\rho_f^0 c_s^0 (\boldsymbol{v}_f - \boldsymbol{v}_s)}{\tau}, 0, 0_{ij} \right)$$

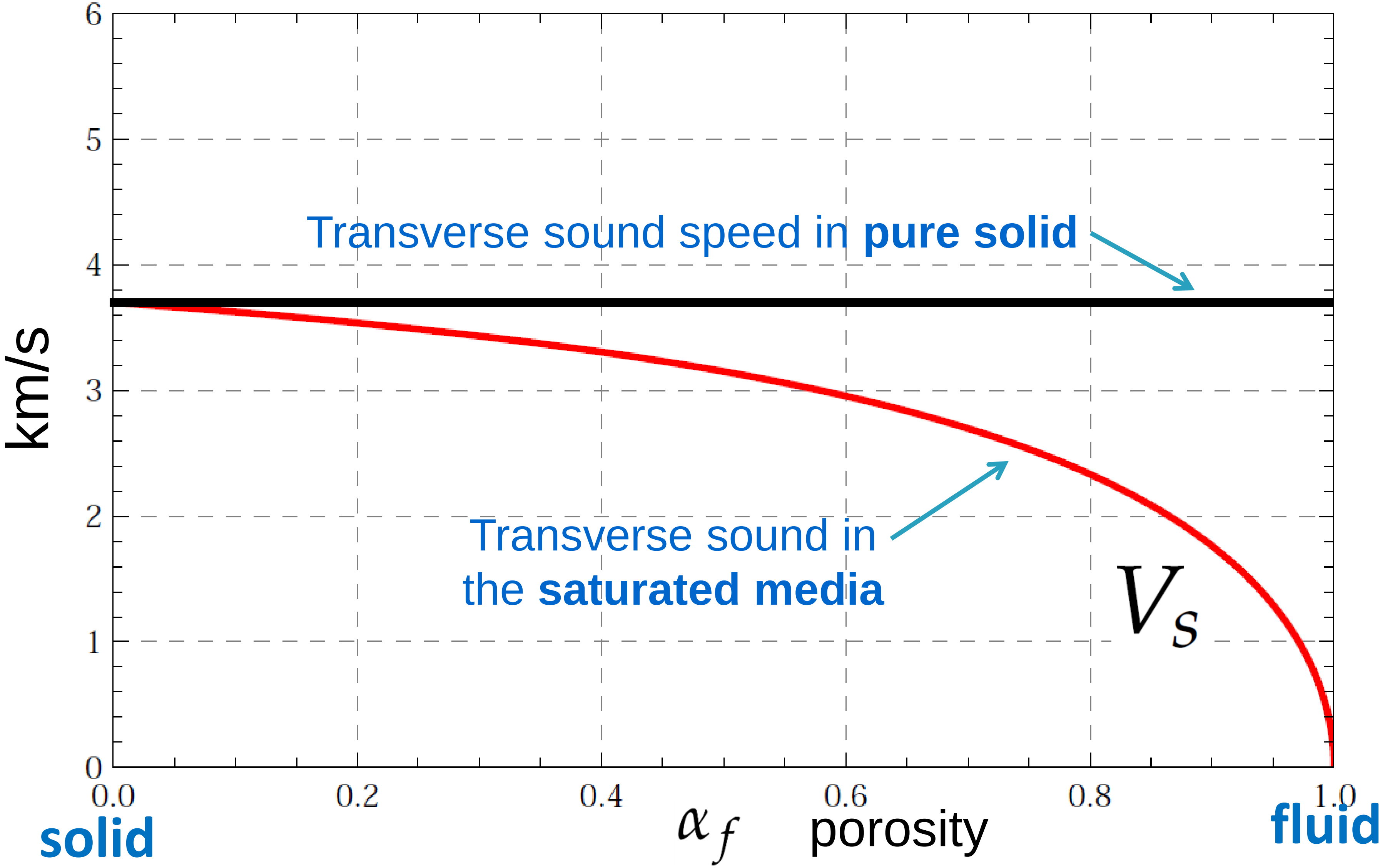
α_s Volume fraction of the solid matrix

c_s **Mass fractions (concentrations)**

Two Longitudinal sound waves (P-waves)



Transverse sound wave



Conclusion

- Hyperbolic (**wave theory**) for viscous, heat and mass transport
- The **unified model** can describe **fluids and solids** in a single system of PDEs
- The model was implemented in the **ADER-FVM-DG** code and tested on a large number of test cases
- Nonlinear solid-fluid mixture model was presented. Application to poroelasticity is expected

Thank you for your attention