Χαμηλοί ρύποι - υψηλές αποδόσεις και ο ρόλος της τυχαιότητας

K. Vogiatzaki

City University, Department of Mechanical Engineering, London, U.K.

Research Trajectory

•**Brighton University, London,UK**
Senior Lecturer (September 2016-)

•**City University, London, UK**
Lecturer (September 2013-To Date)
Key research areas: Engine modelling, Two-Phase Flow modeling, Porous media

•**Massachusetts Institute of Technology,** Cambridge, USA
Research Associate (January 2012 – To Date)
Key research area: Energy production from conventional and renewable resources, focus on combustion instabilities

•**Imperial College of London,** London, UK
Research Associate (January 2010 – December 2011)
Key research areas: Spray modeling for realistic combustors

•**Universität Stuttgart,** Stuttgart, Germany
Research Assistant (February 2009 – December 2009)
Key research areas: Turbulent mixing through Lagrangian modeling

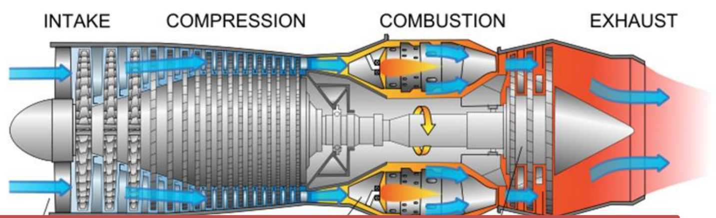
•**Imperial College of London,** London, UK
PhD (October 2005 – February 2009)
Key research areas: Development of a new turbulent combustion model (MMC)

•**National Technical University of Athens,** Athens, Greece
B.Sc plus Master (September 1999 – February 2005)
Majoring in stochastic calculus

Research Focus

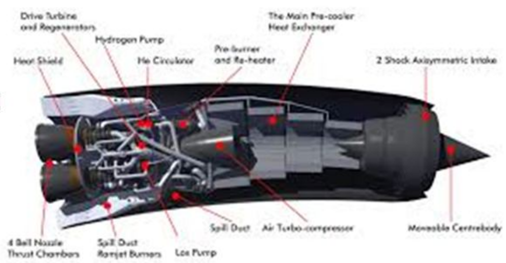
Develop the numerical tools that will help the design of a clean flexible energy systems

Varying fuels (LNG,NG,Syngas,Diesel,Gasolin, combination)



HIGH COMPLEXITY

Varying Inlet Conditions



Stability

Minimum emissions

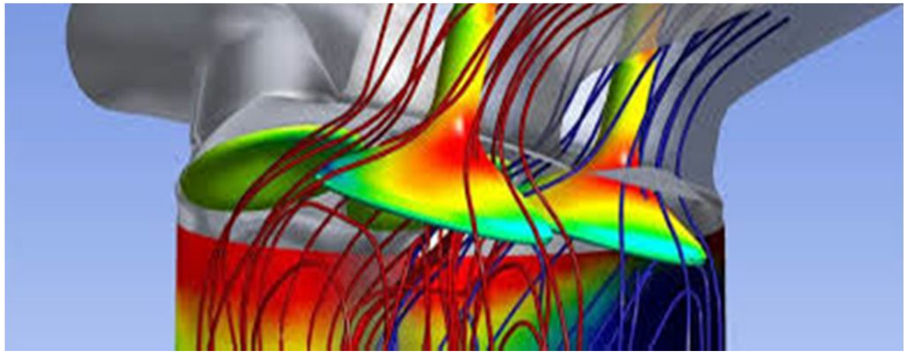
Efficienc
y

Skills: Fluid Dynamics, Modelling Stochasic processes, Material Properties, solution of ODE, programming

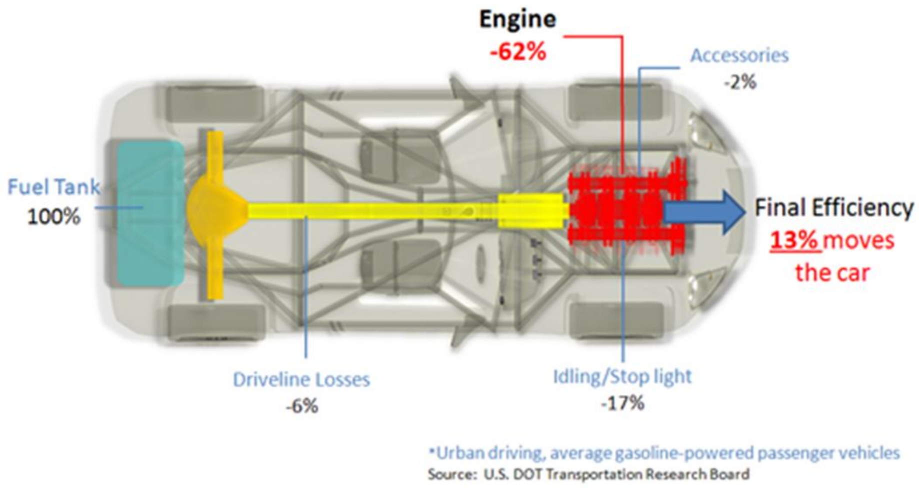
How does it translate to day to day basis?

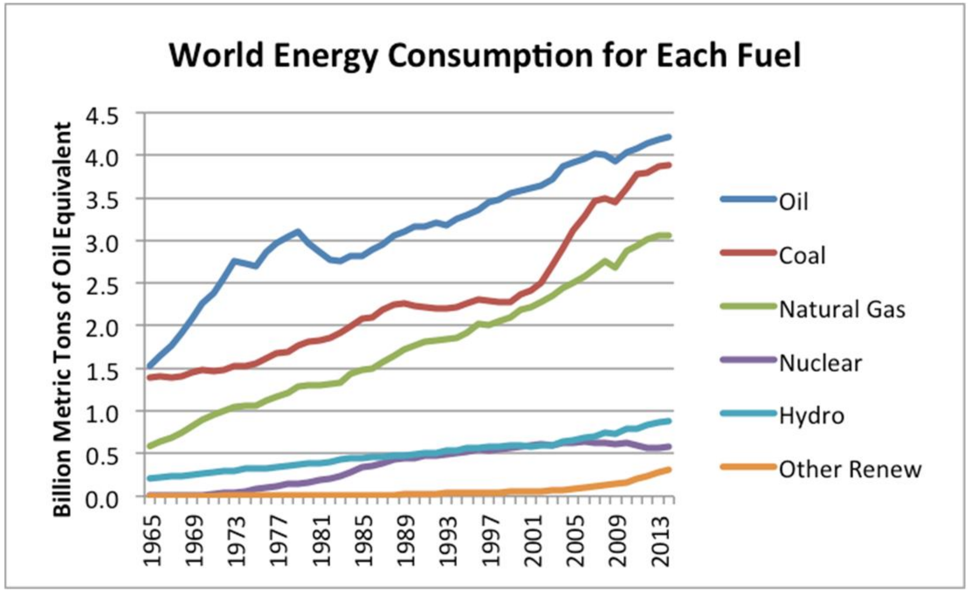
Programming
Fluid Mechanics
Maths

Computational Fluid Dynamics

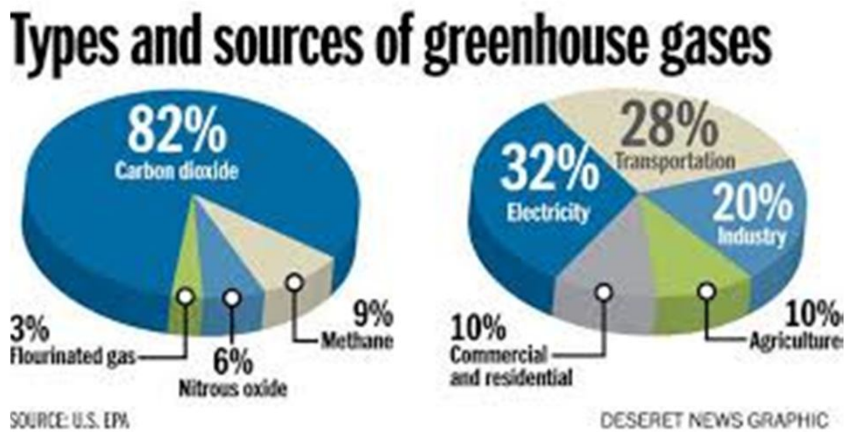


Isn't the existent technology enough?





2015 United Nations Climate Change Conference: The expected key result was an agreement to set a goal of limiting global warming to less than 2 degrees Celsius (° C) compared to pre-industrial levels. The agreement calls for zero net anthropogenic greenhouse gas emissions to be reached during the second half of the 21st century



Goals for the future

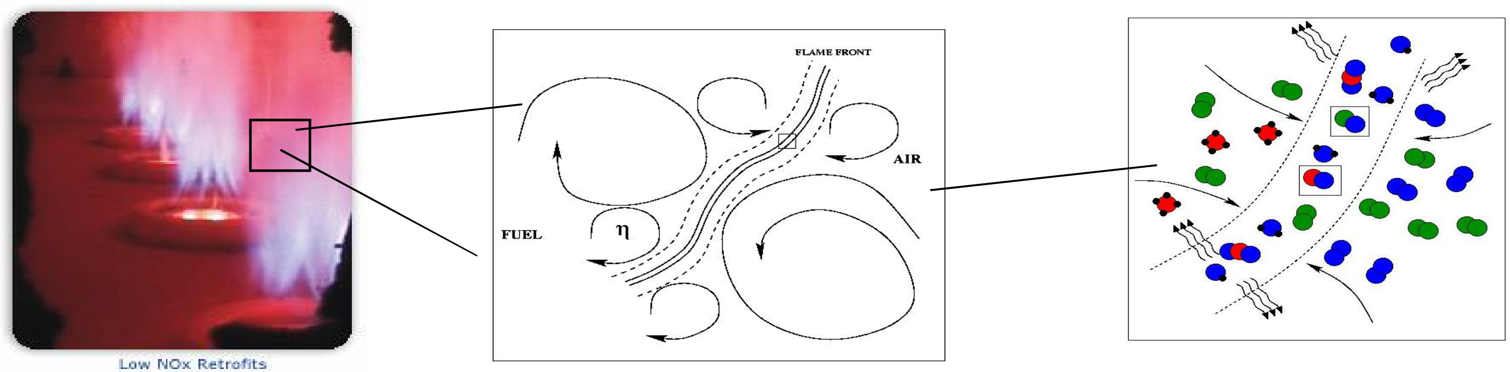
Combustion : Latin.
***Combustionem* which means ''burning''**
+
Engine: Latin *ingenium*: innate quality, a ''clever invention''
=
Burn in a 'clever' way
(more efficient&safe, less polluting, minimum cost)

Where do maths come into picture?

Turbulent Combustion

Combustion modelling
- Mixing of fuel and oxidiser
- Chemistry

Complicated problem (multi-phase multi scale)
-Turbulence: Random Process with chaotic behavior
- Combustion: chemical kinetics, need for efficiency, reduced emissions
- Interaction: Turbulence increases mixing and enhances combustion / Combustion releases heat, which generates flow instability through gas expansion and buoyancy, thus enhancing the transition to turbulence



How do we approach the problem?

(The same way as we do with all physical problems)

a) Level of reality we represent

<u>Molecular level:</u> definition of a discrete system governed by Boltzman equations

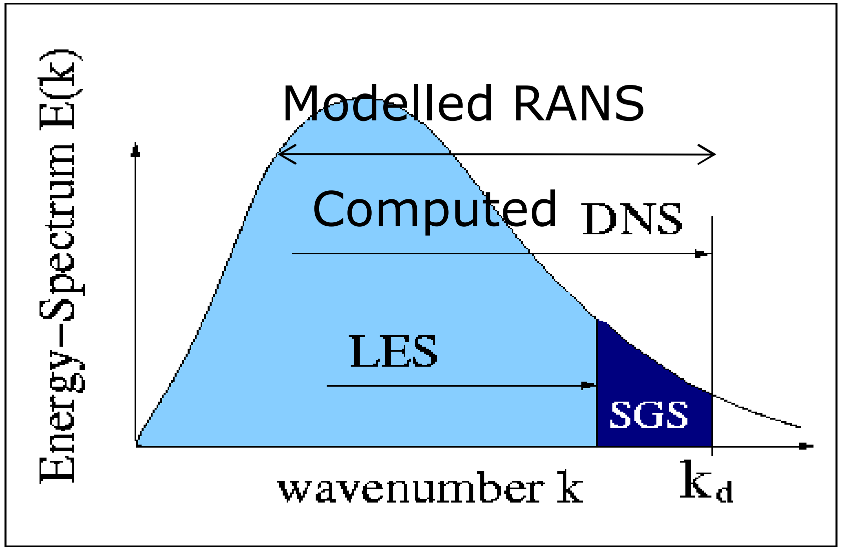
<u>Continuum paradigm:</u> macroscopic description corresponding to a scale of representation larger than the mean free path of the molecules. The system is governed by the Navier Stokes equations

Continuity: $$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

Momentum: $$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i u_j) + \frac{\partial p}{\partial x_j} = \frac{\partial \tau_{ij}}{\partial x_j}$$

Species: $$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = -\frac{\partial}{\partial x_i}(V_{k,i} Y_k) + \omega_k$$

b) Level of time and space resolution



RANS (Averaging):

$$\overline{Y}(x,t) = \frac{1}{T}\int_0^T Y(x,t)\,dt$$

LES (Filtering):

$$\overline{Y}(x,t) = \int_{-\infty}^{+\infty} Y(x,t)F(x-x')\,dx'$$

c) Modelling of unresolved quantities

Turbulence modelling:

Reynolds Stresses: $\overline{u'_i u'_j}$

Species Turbulent fluxes $\overline{u'_i Y'}$

Combustion modelling:

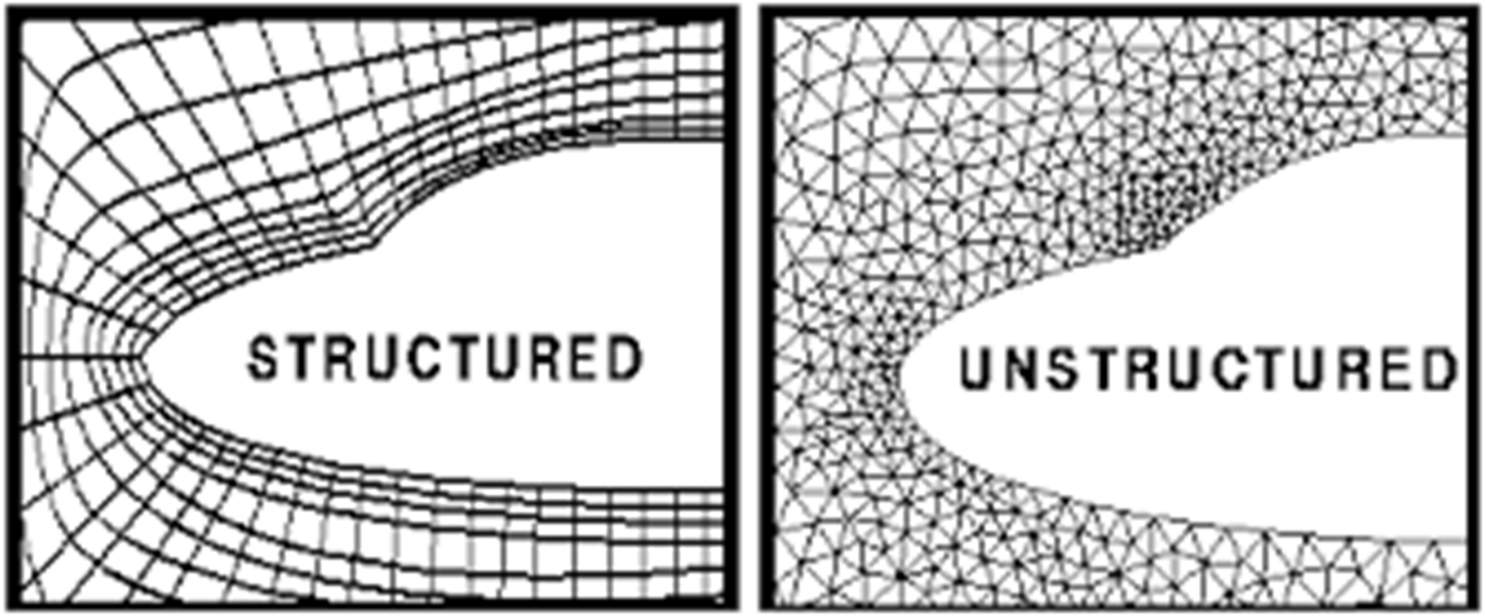
$$F + sO \rightarrow (1+s)P$$

$$\omega_F = -A\rho^2 \mathrm{T}^{\beta} \mathrm{Y}_F Y_o \exp\left(-\frac{T_A}{T}\right)$$

Problem!!!

$$\overline{\omega}(Y) \neq \omega(\overline{Y})$$

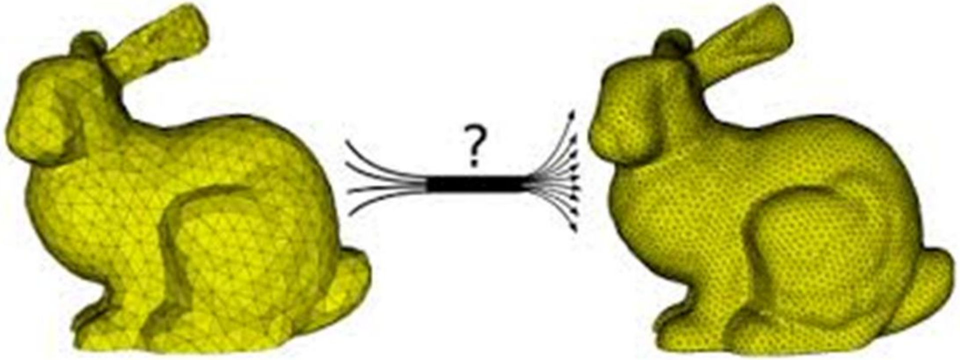
$$\dot{\omega}(\xi) \approx \dot{\omega}(\overline{\xi}) + \left.\frac{\partial \omega}{\partial \xi}\right|_{\xi=\overline{\xi}} \delta\xi + \frac{1}{2} \left.\frac{\partial^2 \dot{\omega}}{\partial \xi^2}\right|_{\xi=\overline{\xi}} (\delta\xi)^2 + \ldots$$

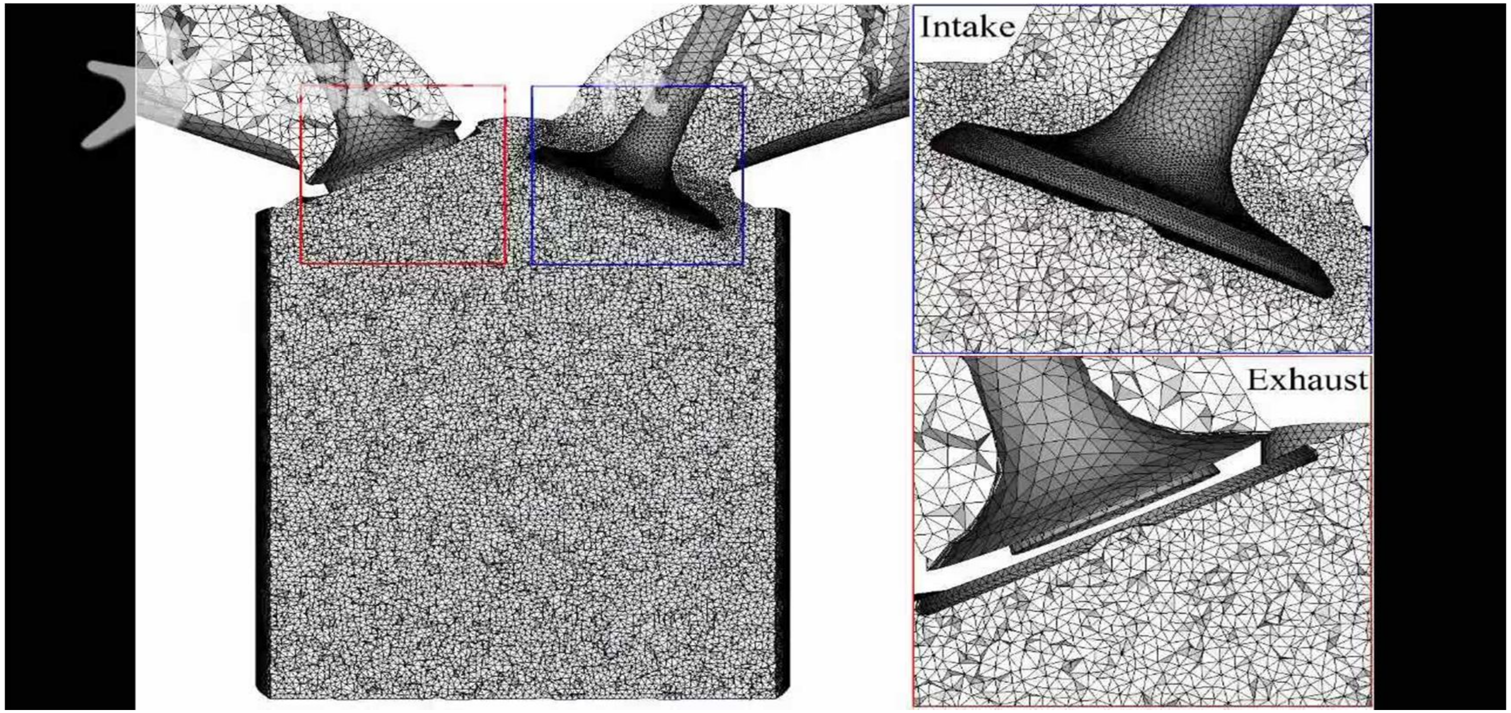


Discretization method (PDE-> ODE)

Mesh: RANS (independent of mesh size, LES (mesh determines resolved scales))

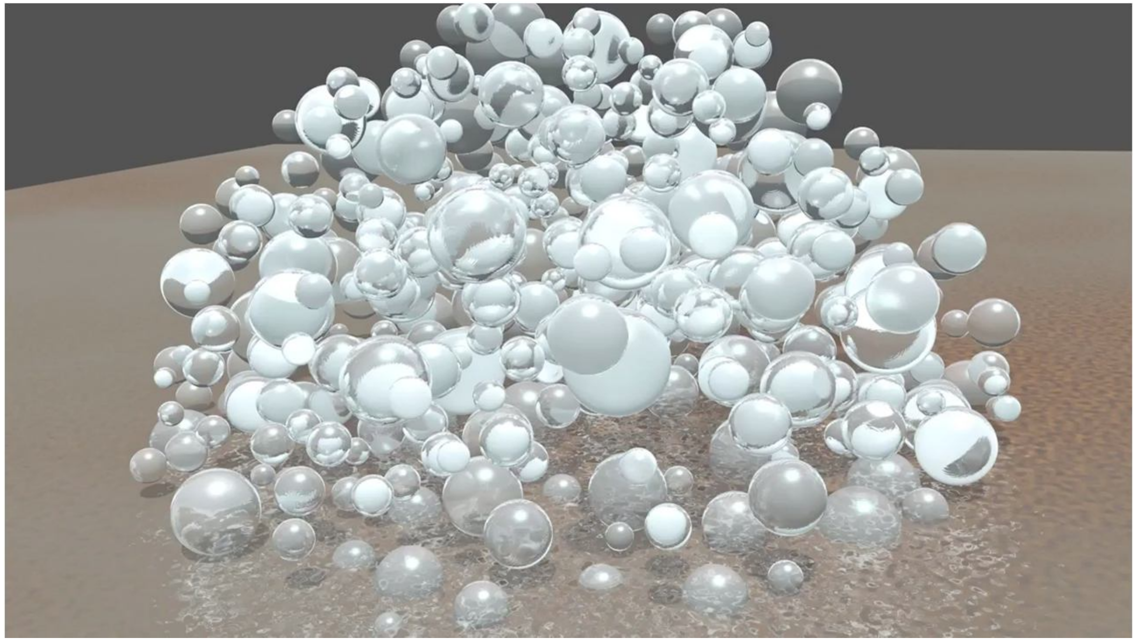
Mesh-Free: Notional particles $\overline{Y}(x,t) = \frac{1}{N}\sum_{1}^{N} Y(x,t;n)$


?


Intake
Exhaust

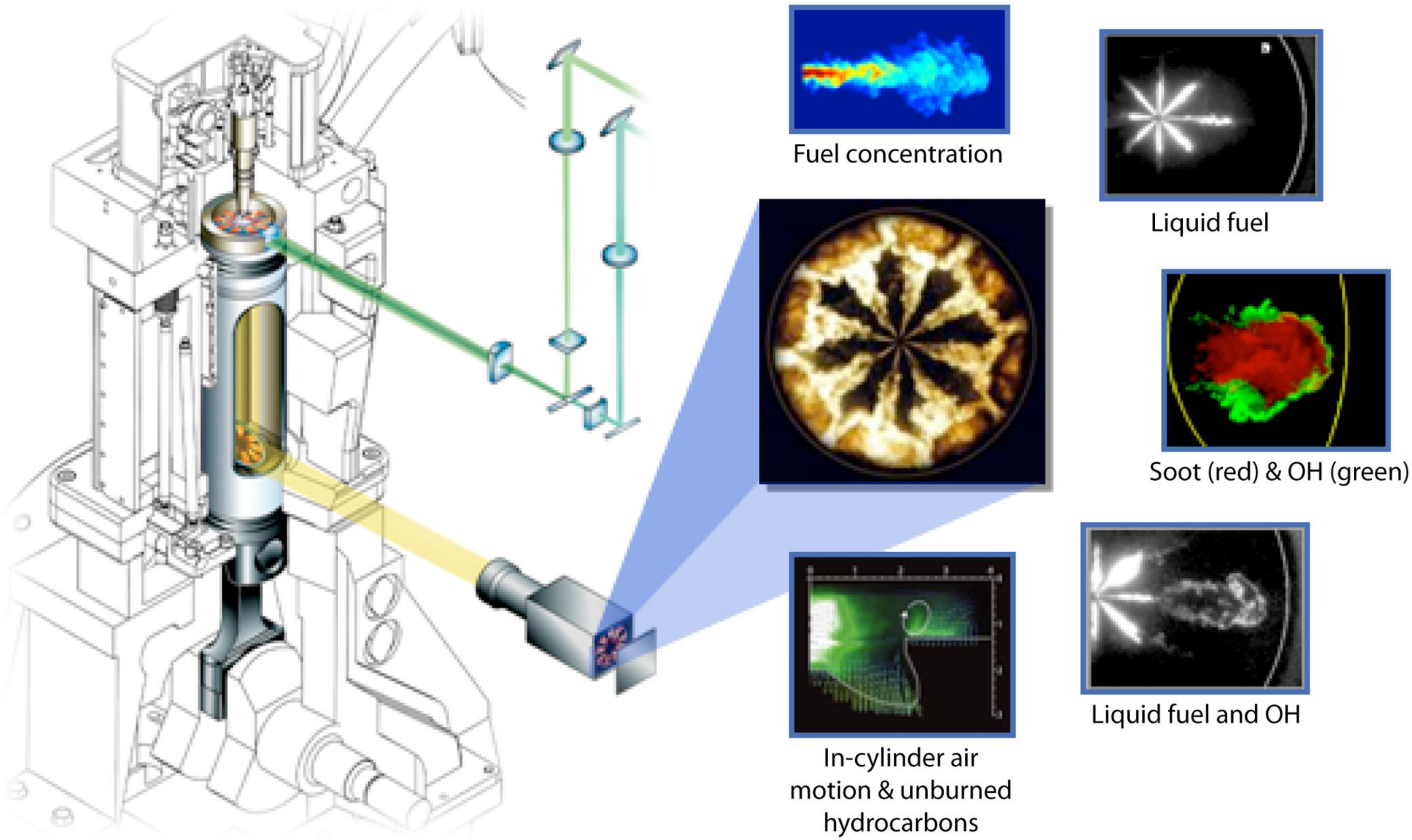
Programming

Programming

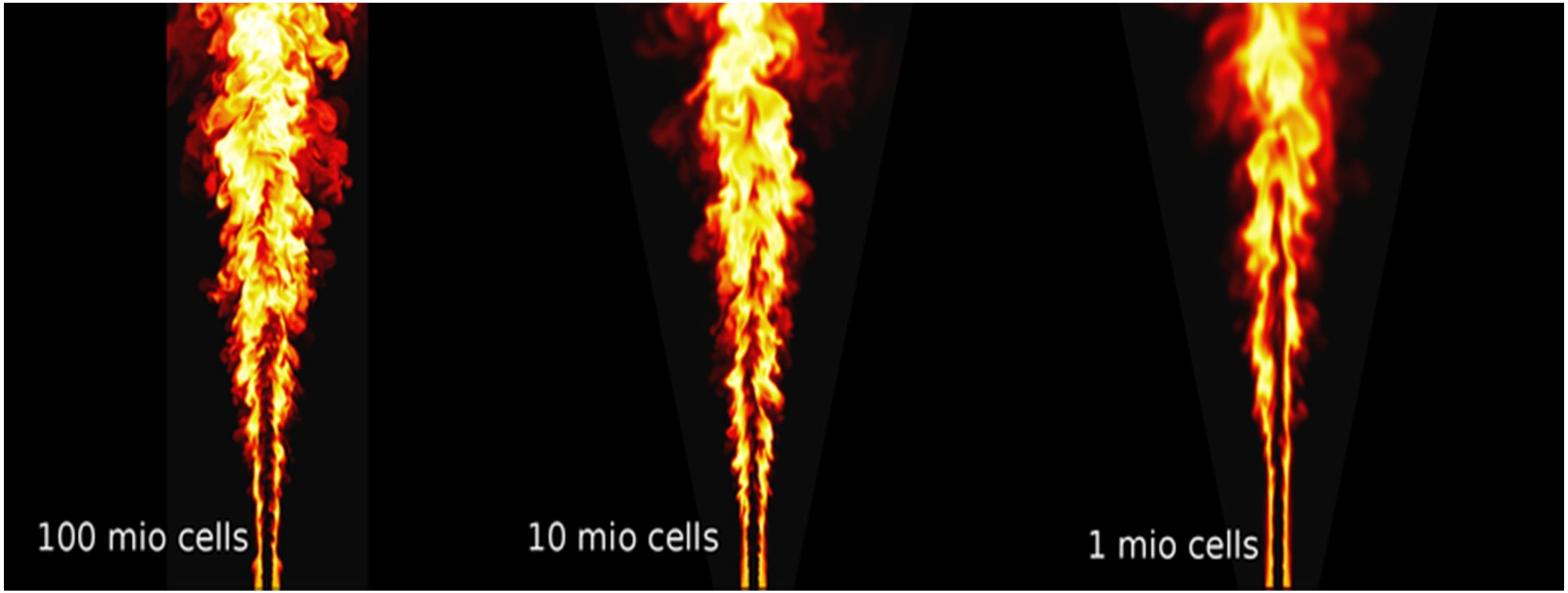


“11 PFLOP/s Simulations of Cloud Cavitation Collapse,” by Diego Rossinelli, Babak Hejazialhosseini, Panagiotis Hadjidoukas and Petros Koumoutsakos, all of ETH Zurich, Costas Bekas and Alessandro Curioni of IBM Zurich Research Laboratory, and Steffen Schmidt and Nikolaus Adams of Technical University Munich.

The researchers, broke some serious computational fluid dynamics ground in their simulation, which maneuvered ***6.4 million threads*** *on the IBM Sequoia system. The simulation, according to IBM, stands as the “largest simulation ever in fluid dynamics by employing* ***13 trillion cells*** *and reaching an unprecedented, for flow simulations, 14.4 petaflop sustained performance on Sequoia—73% of the supercomputer’s theoretical peak*

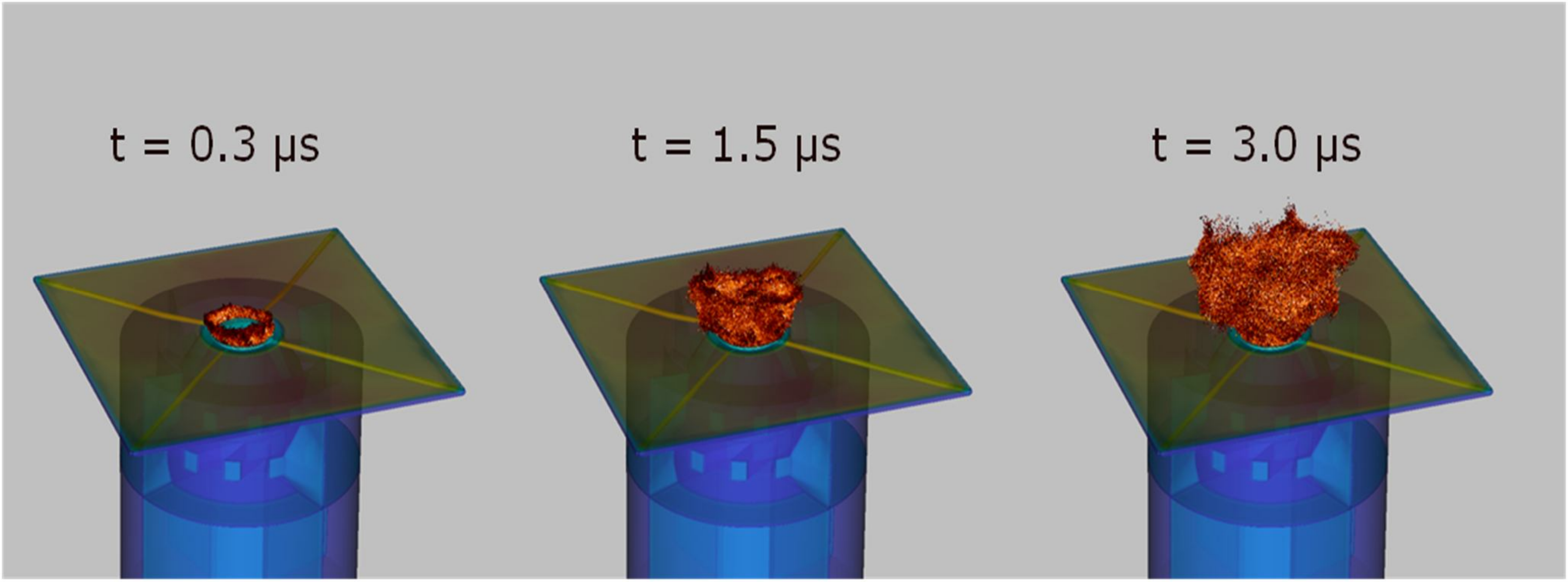

Fuel concentration
Liquid fuel
Soot (red) & OH (green)
In-cylinder air motion & unburned hydrocarbons
Liquid fuel and OH

Flames

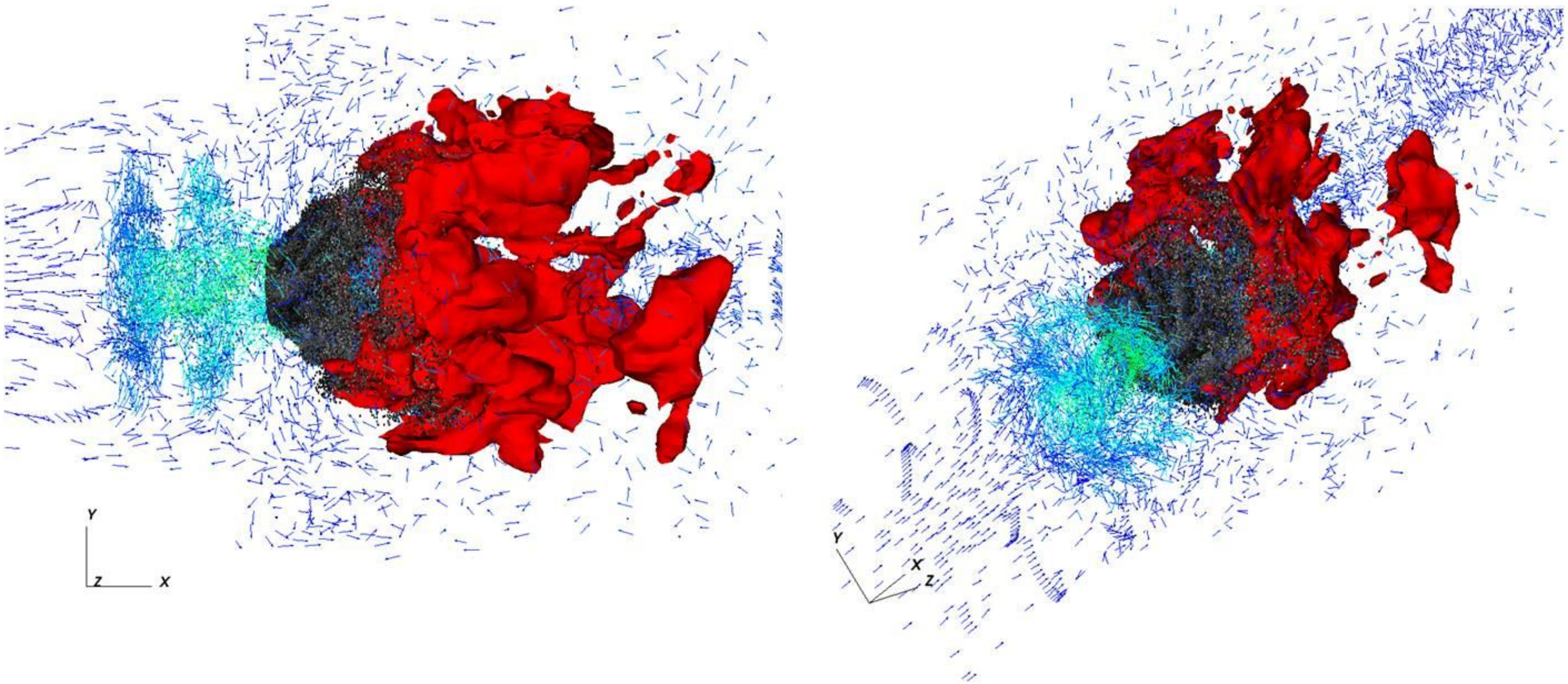


Injection

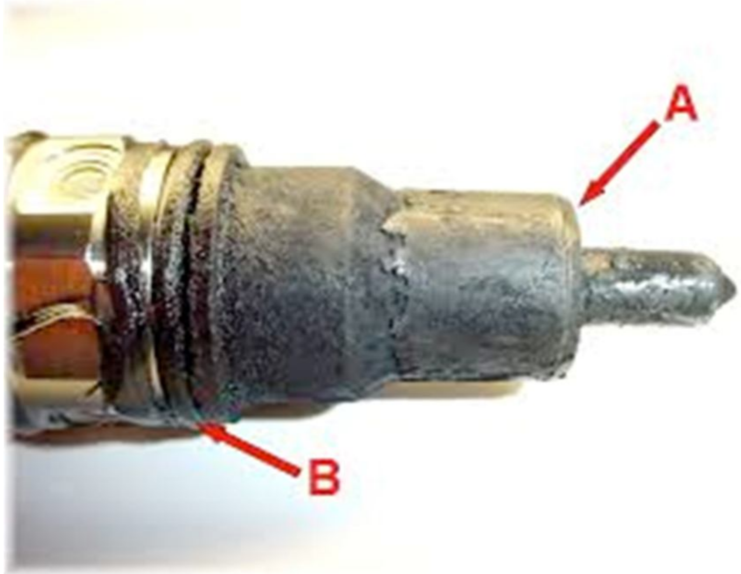
Injection



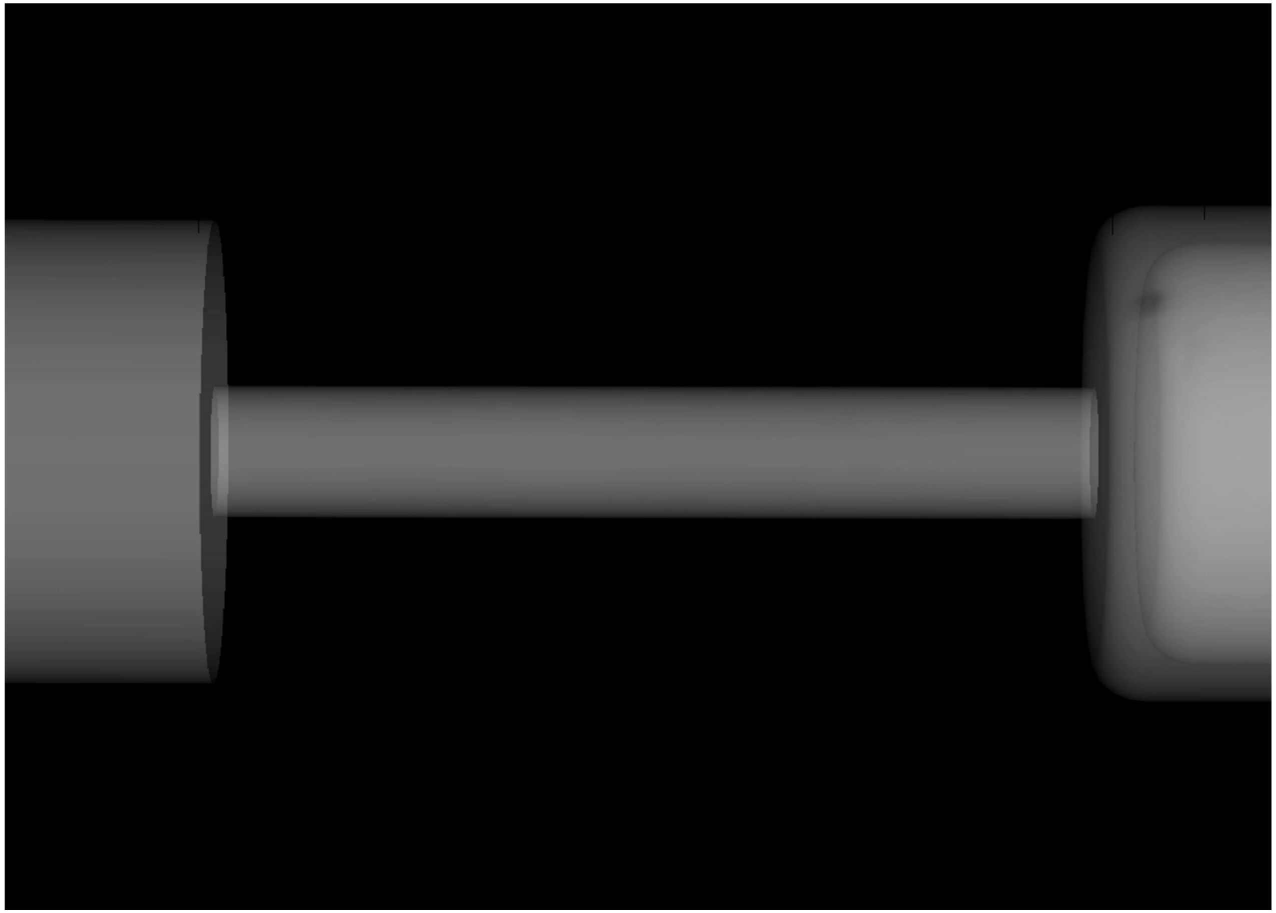
Flame Turbulence Interaction



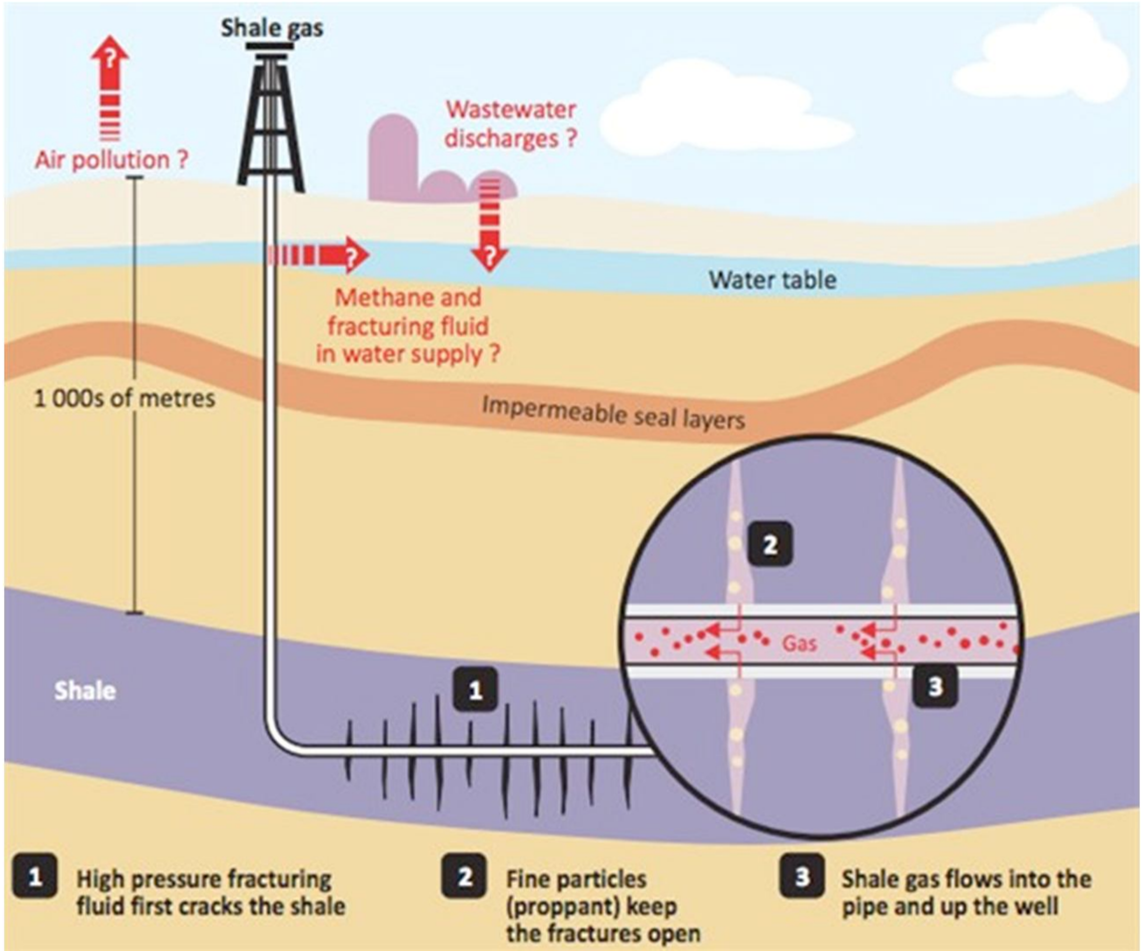
Cavitation



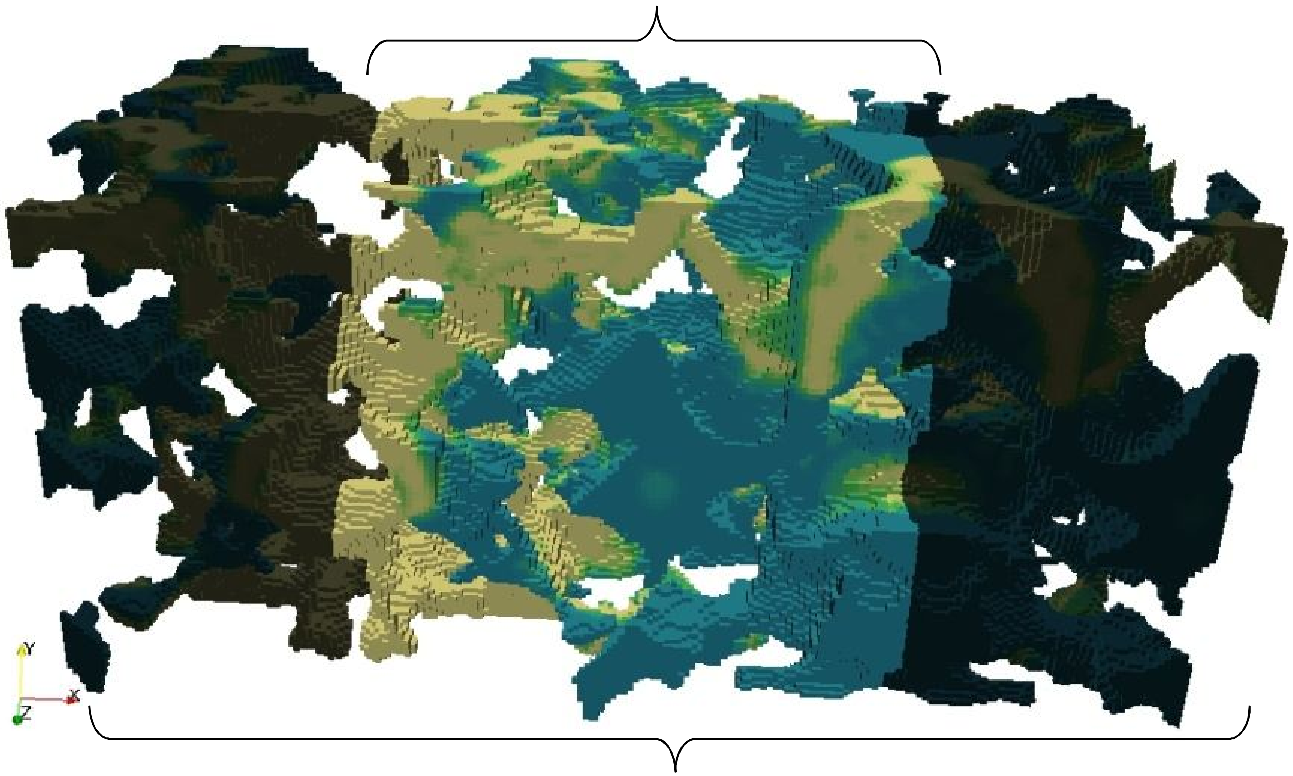
Cavitation



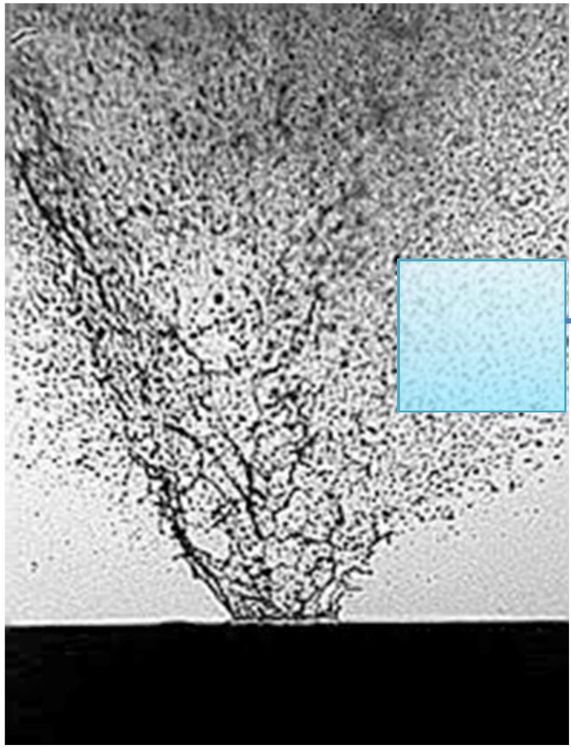
Flows Through Porous Media

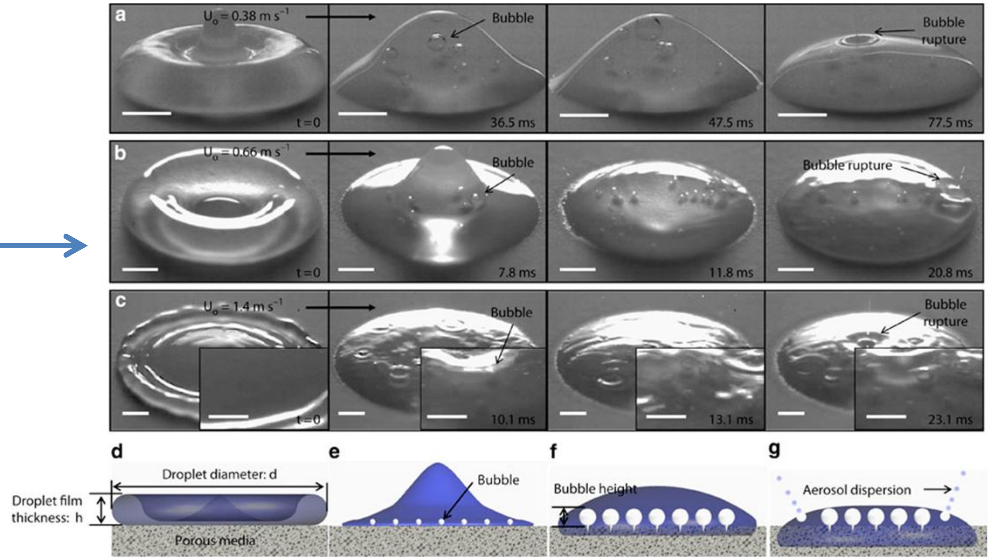


Flows Through Porous Media

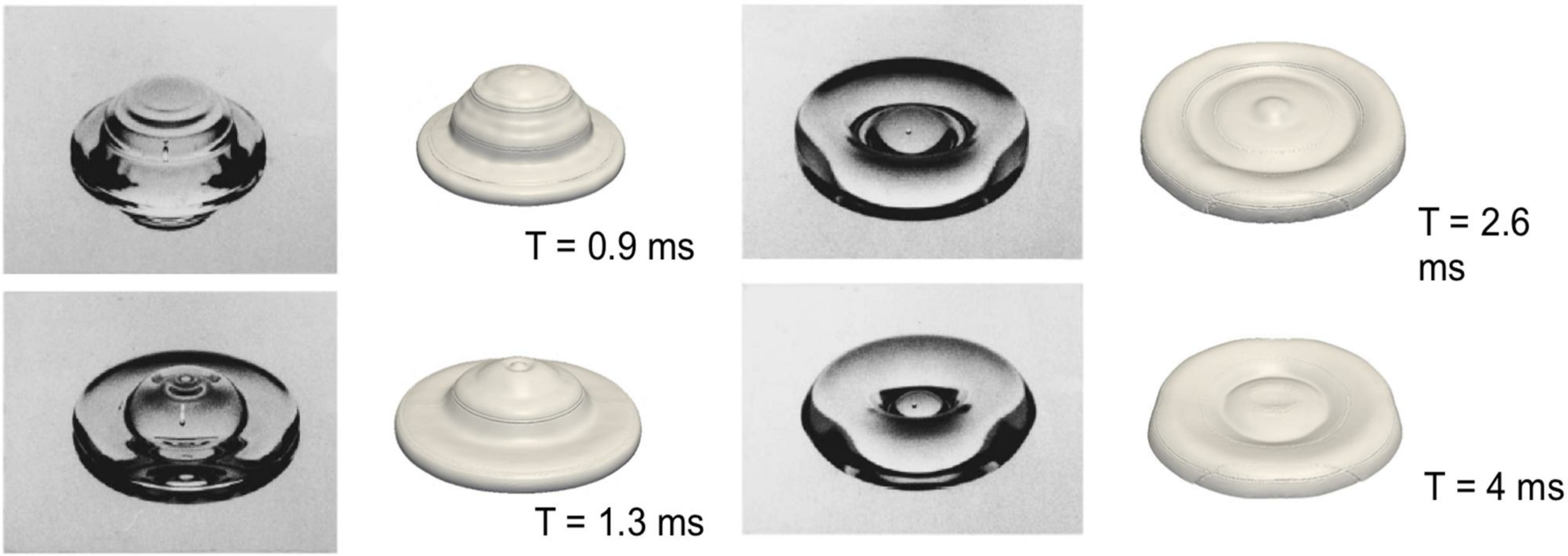


Droplet Impacting Porous Media

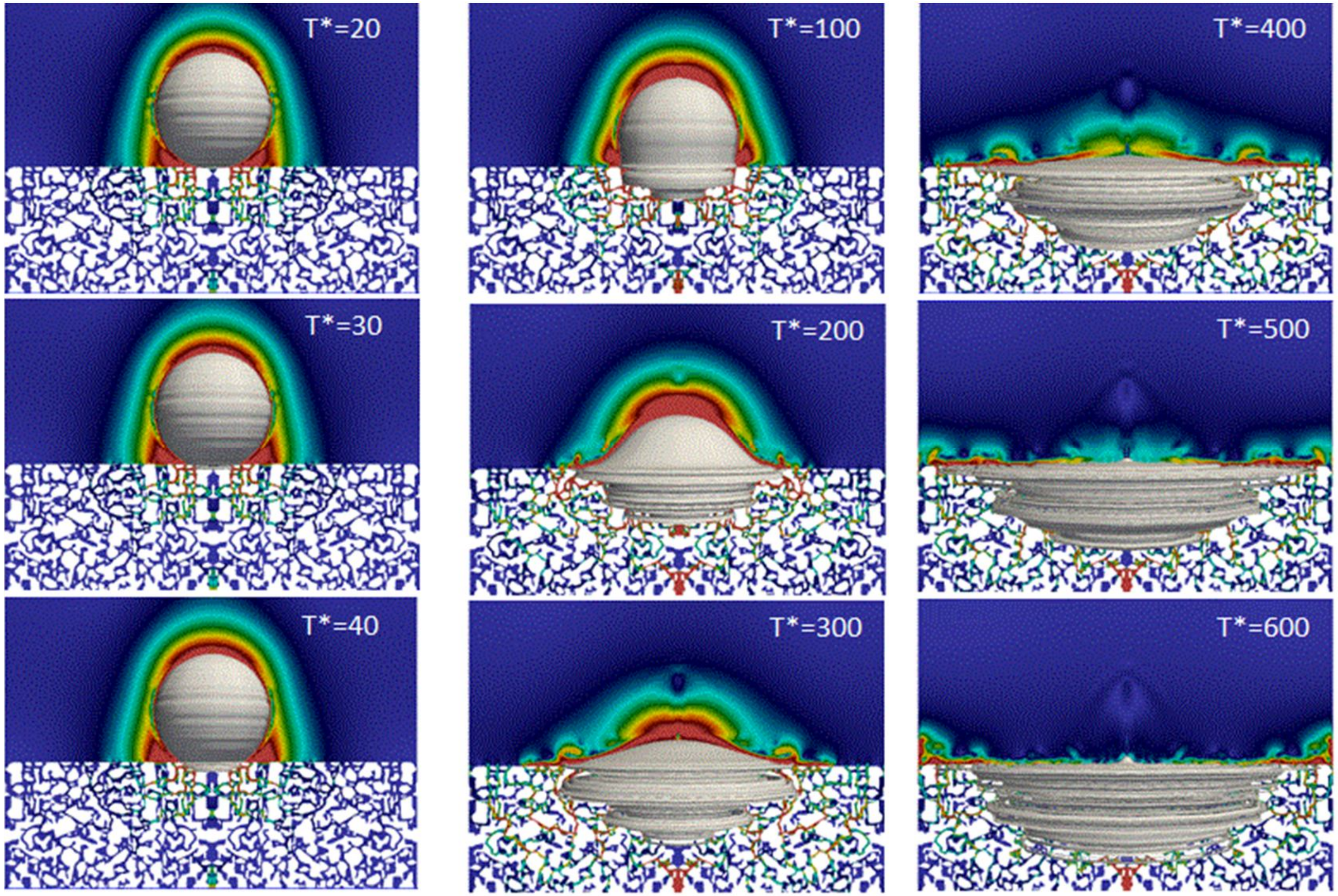




Droplet Impacting Solid Surfaces



Droplet Impacting Porous Media



Good Luck!!!!!!

MMC

MMC CONCEPT: Distinguishing major and minor fluctuations of species

SPECIES

$$\frac{\partial \rho Y_l}{\partial t} + \nabla \cdot (\rho v Y_l) - \nabla \cdot (\rho D \nabla Y_l) = W_l \quad l = 1,2\ldots,\ n_s$$

COMBINE

PDF CONCEPT

Major Species: Fluctuations of this set are not restricted.

$$\tilde{P}_Y = \tilde{P}_{Y_{major}}$$

$$\frac{\partial \langle \rho \rangle \tilde{P}_Y}{\partial t} + \nabla \cdot (\mathbf{u} \langle \rho \rangle \tilde{P}_Y) + \frac{\partial W_I \langle \rho \rangle \tilde{P}_Y}{\partial y_I} + \frac{\partial N \langle \rho \rangle \tilde{P}_Y}{\partial y_I \partial y_J} = 0$$

CMC CONCEPT

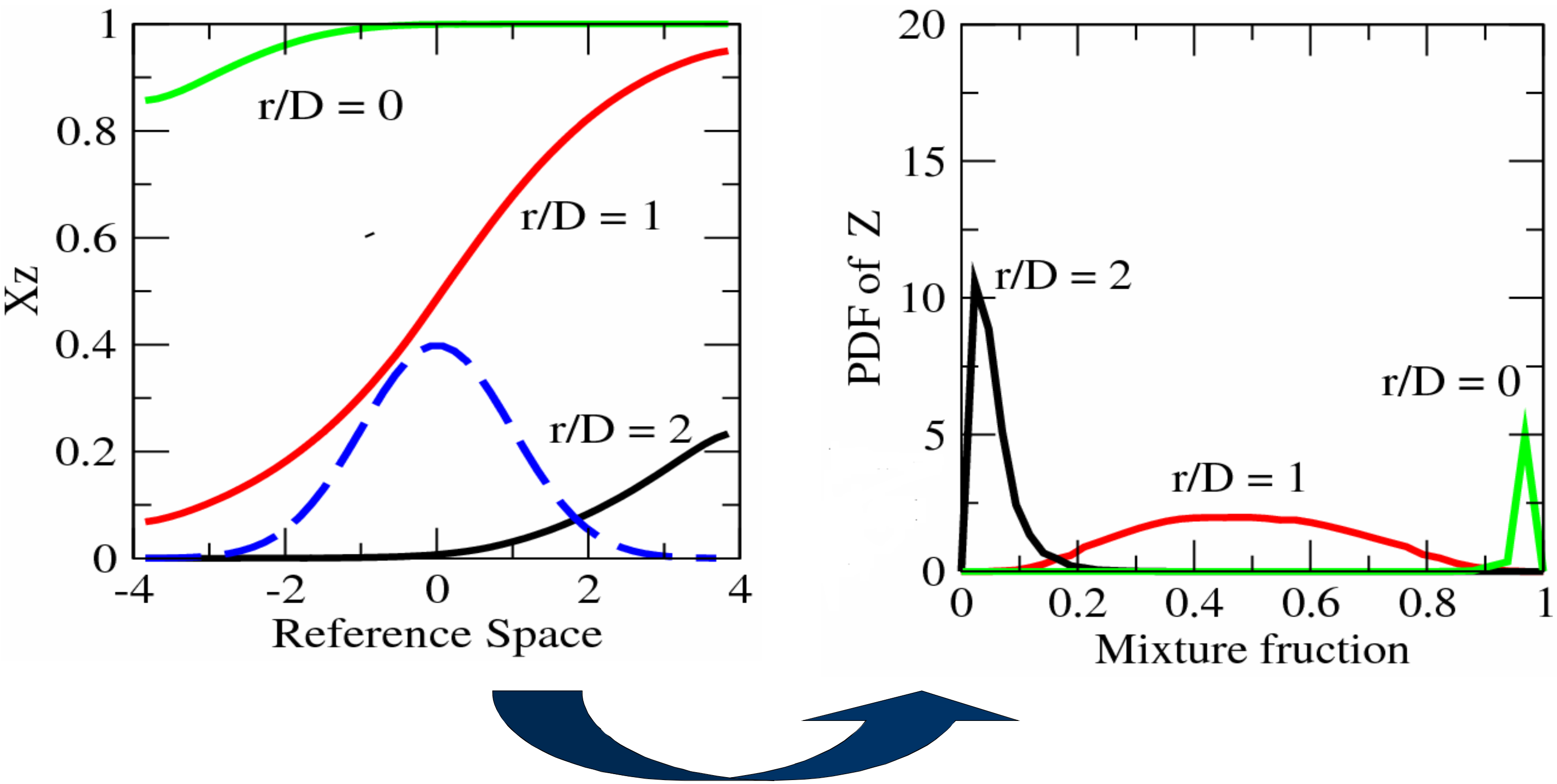
Minor Species: Are allowed to fluctuate only jointly with major species.

$$Q_a = \langle Y_{\min or} \mid Y_{major} \rangle$$

$$\frac{\partial Q_a}{\partial t} + \mathbf{u} \cdot \nabla Q_a + W_i \frac{\partial Q_a}{\partial y_i} - N \frac{\partial^2 Q_a}{\partial y_i \partial y_j} = W_a$$

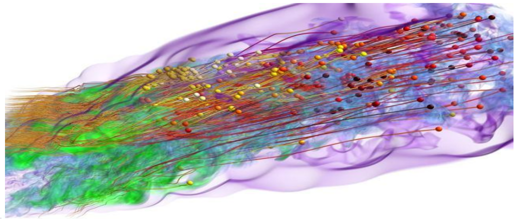
Mapping Closure Concept

Concept: The fluctuations of the major species are modeled by the fluctuations driven by the oscillations of the stochastic reference field.



Xz is the mapping function between the Gaussian reference space and the mixture fraction (Z) space

The Particle Method



Particle Method:
Notional particles= Monte Carlo numerical algorithm in order to solve PDF transport equation.

$$\frac{\partial F}{\partial t} + \frac{\partial A^i F}{\partial x^i} - \frac{\partial^2 B^{ij} F}{\partial x^i \partial x^j} = 0$$

Kolmogorov Forward equation

$$\frac{\partial P}{\partial t} + \frac{\partial \hat{u}_i P}{\partial x_i} + \frac{\partial \hat{A}_I P}{\partial z_I} + \frac{\partial^2 B_{IJ} P}{\partial z_I \partial z_J} - D\frac{\partial^2 P}{\partial x_i \partial x_i} = 0$$

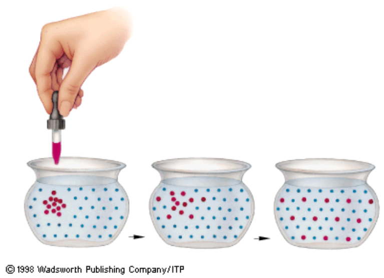
$$\mathrm{d}x_p^i = A^i(\mathbf{x}_p, t)\,\mathrm{d}t + b^{ij}(\mathbf{x}_p, t)\,\mathrm{d}w_p^j$$

Ito

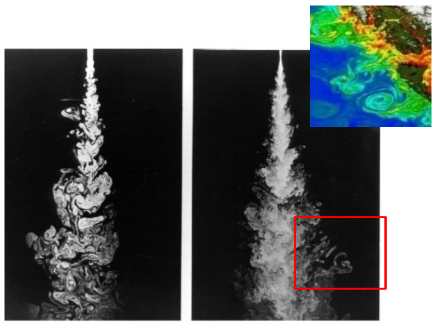
$$\mathrm{d}x_p^i = A^i(\mathbf{x}_p, t)\,\mathrm{d}t + b^{ij}(\mathbf{x}_p, t)\,\mathrm{d}w_p^j$$

$$\frac{dZ_p^{(\alpha)}}{dt} = W_p^{(\alpha)} + \left[\frac{dZ_p^{(\alpha)}}{dt}\right]_{\mathrm{mix}}$$

Physical Diffusion



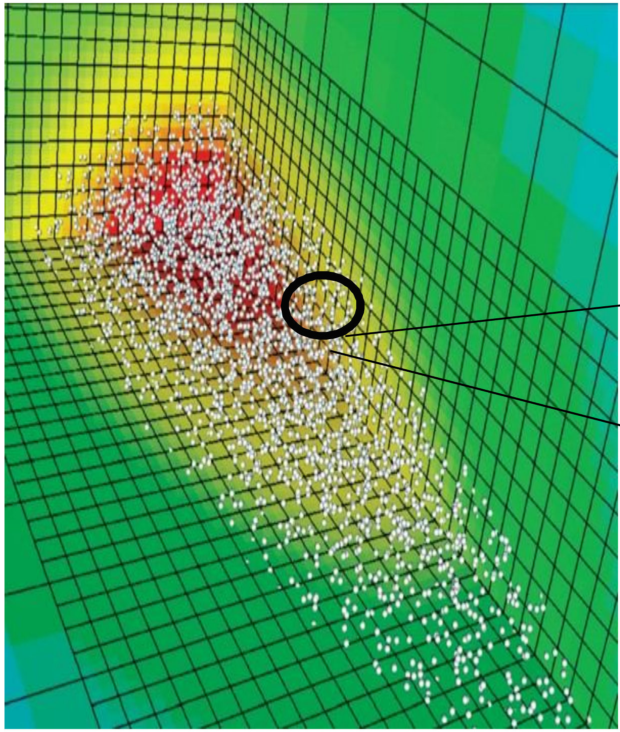
Turbulent Diffusion

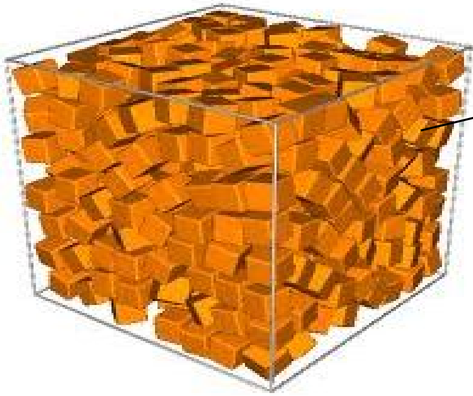


Mathematical Model
Particle-to-cell mixing
(we 'mix' random variables)

Specific Application:
Turbulent Mixing
(accelerates the homogenization of any non-uniform fluid mixture)

Mixing Model





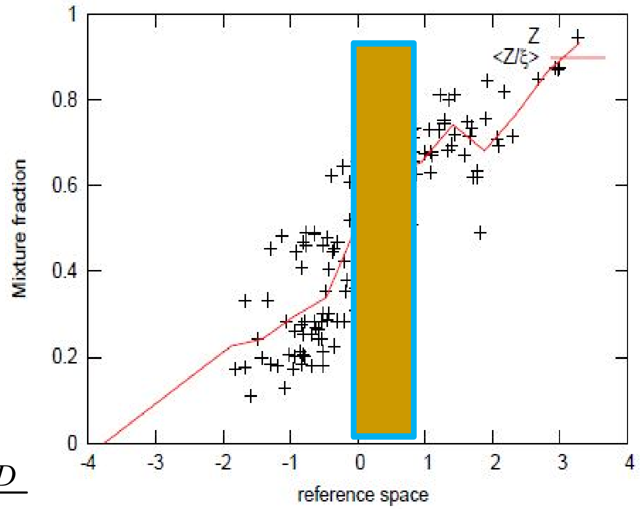
Each particle 'carries' information for the chemical composition at this cell

$$\frac{dZ_p^{(\alpha)}}{dt} = W_p^{(\alpha)} + \left[\frac{dZ_p^{(\alpha)}}{dt}\right]_{\text{mix}}$$

Mapping Closure Idea IDEA!!

Each particle 'carries' information for the chemical composition at this cell + reference space

$$d\xi^p = A(\xi^p, x^p, t)dt + B(\xi^p, x^p, t)dw$$



$$y^{(p)new} = y^{(p)} + \frac{1}{\tau_Y}(< y \mid \xi > - y^{(p)})$$ MMC - IEM

$$y^{(p)new} = y^{(p)} + \frac{1}{\tau_Y}(y^{(q)} - y^{(p)}) \Rightarrow$$ MMC - Curl

$$\tau_Y = \frac{\tau_D}{C_Y}$$

Energy ~ Combustion Systems