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Plenary Session on Computational Science and Engineering
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Survey on Adaptive Finite Volume in Engineering and Science: Computational Fluid Dynamics in Industry

Fayssal Benkhaldoun - Adaptive Finite Volume Method in CFD

LAGA - PRES Sorbonne Paris Cité - France

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The objective of this presentation is to introduce a survey on efficient numerical methods for stiff problems in computational fluid dynamics. In particular, developing an adaptive finite volume black-box has become one of the active research fields worldwide. In this survey we present a review on recent advances in adaptive finite volume methods for industrial applications. More precisely, we discuss the application of this class of methods to the following situations:

- Combustion
- Plasma Physics
- Flows in porous media

GENERAL INTRODUCTION

The first part of this talk presents a combustion problem where we address the numerical simulation of a triple flame ignition. This phenomena is of great importance for car design industries among others.

In the second part plasma physics problems are considered. Research in this field is crucial for example for the treatment of contaminated media, for ITER Tokamak safety issues (nuclear industry) and for fast laser assisted combustion in aerospace engineering. Here we focus mainly on a propagation phenomena of the streamer discharge in cold plasma.

The last section of this presentation is focused on practical problems for multiphase flows in porous media. This part of our survey covers engineering problems in petroleum industry as well as the CO₂ storage in confined and unconfined aquifers.

FLAME IGNITION AROUND A DROPLET

in collaboration with Roland Borghi⁺ and Imad Elmahi*

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Introduction

Droplet ignition and burning subject of great interest;
Fuel droplets dispersed in an oxidizing gaseous medium;
Propagation of a flame zone in a premixed spray;
Droplet inflammation: many practical combustion devices;
Liquid-fuelled rocket, diesel engines;
Important impact on the production of pollutants;
Wide range of technological applications;
great interest for safety problems.

Picture of Diesel Engine

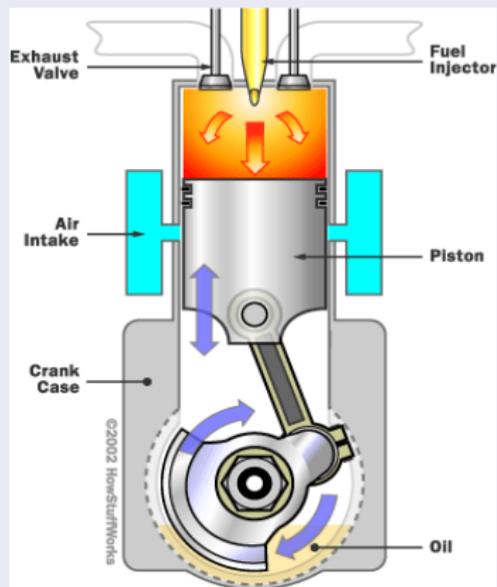


Figure: Diesel Two-Stroke Engine

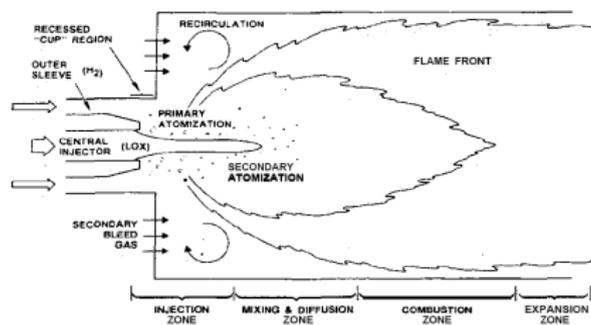


Figure: Combustion chamber

Roland Borghi Triple Flame Conjecture (1994)

Small droplets vaporize the preheating zone;

Spray flame is a classical premixed flame;

Flame propagates towards the unburnt mixture due to the heat and mass diffusion from the burnt gases;

Different situation when time necessary for droplet vaporization is larger than the transit time in the preheated zone;

Liquid large droplets can be found behind the premixed flame;

Premixed flame is broken locally by a droplet surrounded by a mixture too rich to allow a flame to persist.

Roland Borghi Triple Flame Conjecture (1994)

Hence, in many locations, the premixed flamelet is connected with a diffusion flamelet that envelopes a droplet or a group of droplets, showing a so called triple flame.

Burning droplets

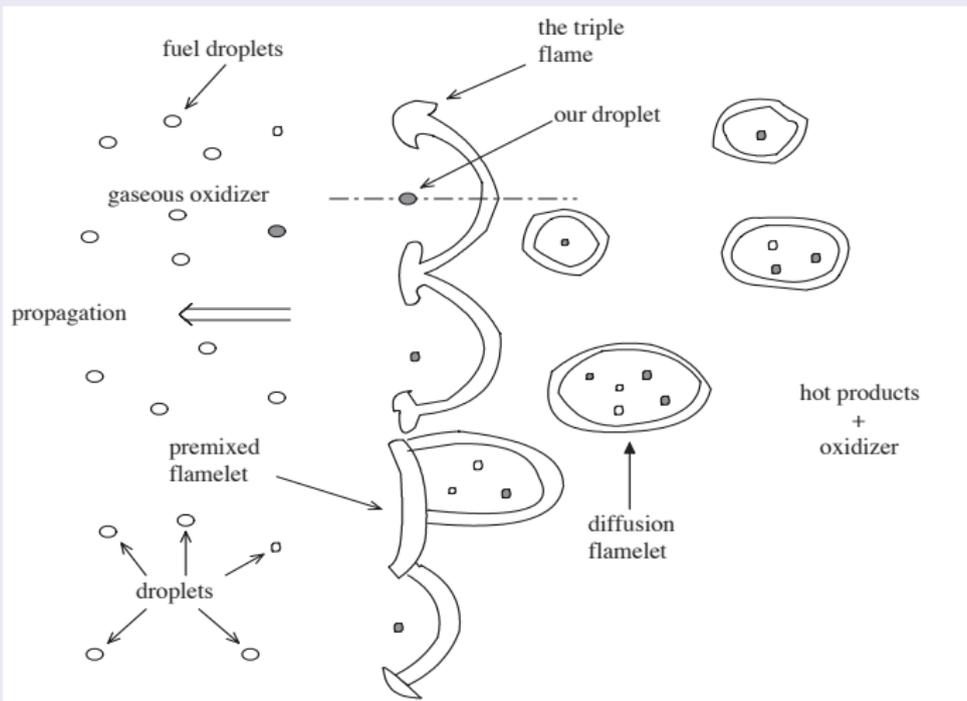


Figure: Burning droplets

Triple flame structure

A triple flame is a flame structure generated by flame propagation in a partially premixed system;

The mixture fraction, Z , determines the burning velocity, s_L ;

The flame in a partially premixed field propagates preferentially along surfaces of stoichiometric mixture, i.e. near $Z = Z_{st}$ where flame speeds are maximum;

The lean and rich premixed flame branches propagate with a lower burning velocity than the leading edge of the flame, called the triple point;

Behind premixed flame front, unburnt intermediates (CO and H₂), and unburnt oxidant, burn as a diffusion flame.

Triple flame structure

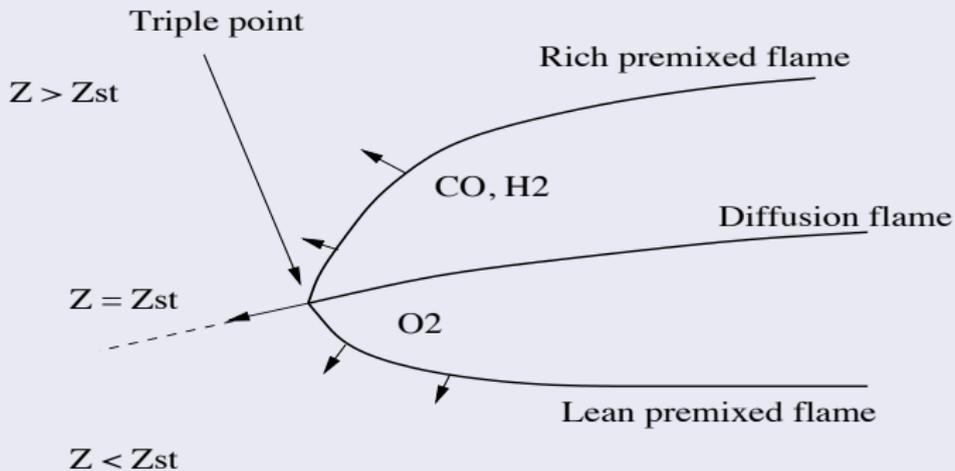


Figure: Triple flame scheme

Triple flame interest

Potential role triple flames play in flame propagation in partially pre-mixed mixtures;

Understanding of stabilization of turbulent diffusion flames;

Role in the ignition processes of non-premixed systems;

Provide information concerning pollutant formation due to large NO_x emissions in turbulent flames.

Combustion proces: one-step overall chemical reaction;



ν : stoichiometric oxidizer/fuel mass ratio;

Model solving equations of continuity, fuel species diffusion, and energy

$$\frac{\partial W}{\partial t} + \frac{\partial(F_{nv} + F_v)(W)}{\partial x} + \frac{\partial(G_{nv} + G_v)(W)}{\partial y} = S(W) \quad (1)$$

$$W = (\rho, \rho u, \rho v, E, \rho Y_F, \rho Y_O)^t,$$

$$F_{nv}(W) = (\rho u, \rho u^2 + P, \rho uv, (E + P)u, \rho u Y_F, \rho u Y_O)^t,$$

$$G_{nv}(W) = (\rho v, \rho uv, \rho v^2 + P, (E + P)v, \rho v Y_F, \rho v Y_O)^t,$$

$$F_v(W) =$$

$$\left(0, -\sigma_{xx}, -\sigma_{yx}, -(u\sigma_{xx} + v\sigma_{yx} - q_x), -D \frac{\partial Y_F}{\partial x}, -D \frac{\partial Y_O}{\partial x} \right)^t,$$

$$G_v(W) =$$

$$\left(0, -\sigma_{xy}, -\sigma_{yy}, -(u\sigma_{xy} + v\sigma_{yy} - q_y), -D \frac{\partial Y_F}{\partial y}, -D \frac{\partial Y_O}{\partial y} \right)^t,$$

$$S(W) = (0, 0, 0, \omega \Delta Q, -M_F \omega, -\nu M_O \omega)^t.$$

Consider the hyperbolic part of the equations (1)

$$W_t + F_{nv}(W)_x + G_{nv}(W)_y = 0 \quad (2)$$

classically called the Euler equations.

Note $\mathcal{F}_{nv}(W, \vec{n}) = n_x F_{nv}(W) + n_y G_{nv}(W)$:

$$\int_{\Gamma_{ij}} \mathcal{F}_{nv}(W, \vec{n}) d\sigma = \Phi(W_i, W_j, \vec{n}_{ij}) \text{meas}(\Gamma_{ij})$$

where Γ_{ij} is the interface between two triangles T_i and T_j .

Roe proposed a particular choice of $\Phi(W_i, W_j, \vec{n}_{ij})$ (Roe 1981):

$$\begin{aligned}\Phi(W_i, W_j, \vec{n}_{ij}) &= \frac{1}{2}[\mathcal{F}_{nv}(W_i, \vec{n}_{ij}) + \mathcal{F}_{nv}(W_j, \vec{n}_{ij})] \quad (3) \\ &- \frac{1}{2}|A(\tilde{W}, \vec{n}_{ij})|(W_j - W_i)\end{aligned}$$

Conservativity condition:

$$\mathcal{F}_{nv}(W_j, \vec{n}_{ij}) - \mathcal{F}_{nv}(W_i, \vec{n}_{ij}) = A(\tilde{W}, \vec{n}_{ij})(W_j - W_i)$$

MUSCL-FVM method

For the first order accurate scheme described above, the values of the variables at a cell face are taken to be the cell-centered values on either side of the face.

The scheme obtained is monotone but has a poor accuracy, due to the large amount of numerical dissipation.

The extension to second order upon unstructured meshes is realized here by supposing that the states are in a set of linear piecewise functions in each control volume, and using the MUSCL technique due to Van Leer (1985).

When discretizing the diffusive part of (1), one has to evaluate term such as

$$\int_{\Gamma_{ij}} \left(a' \frac{\partial a}{\partial x} n_x + b' \frac{\partial b}{\partial y} n_y \right) d\sigma$$

where a (respectively b) is either u , v , T , Y_F or Y_O ; a' (respectively b') is either u , v , P , Y_F or Y_O .

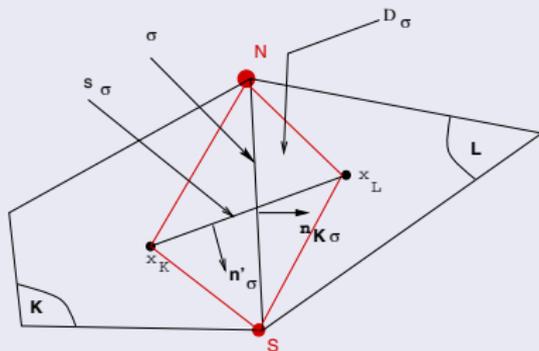
The Green-Gauss divergence Theorem

$$\frac{\partial a}{\partial x} \Big|_{\Gamma_{ij}} \simeq \frac{1}{\text{meas}(C_{dec})} \sum_{\varepsilon \in \partial C_{dec}} \frac{1}{2} (a_{N_1} + a_{N_2}) \int_{\varepsilon} n_{x\varepsilon} d\sigma$$

where N_1 and N_2 are the nodes of an edge ε of ∂C_{dec} . a_{N_1} and a_{N_2} are respectively the values of the state a on the node N_1 and N_2 .

VFdiamond scheme

$$\nabla_{\sigma} u_h = \frac{1}{2|D_{\sigma}|} [(u_L - u_K)|\sigma| \mathbf{n}_{K,\sigma} + (u_S - u_N)|s_{\sigma}| \mathbf{n}'_{\sigma}] .$$



Numerical Investigation

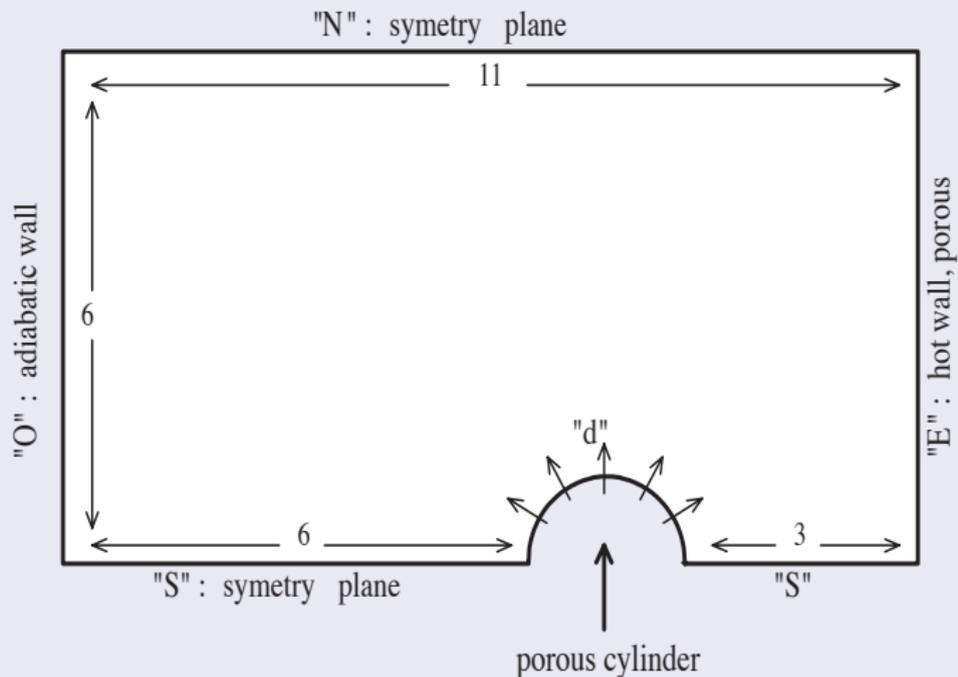


Figure: Simplified configuration

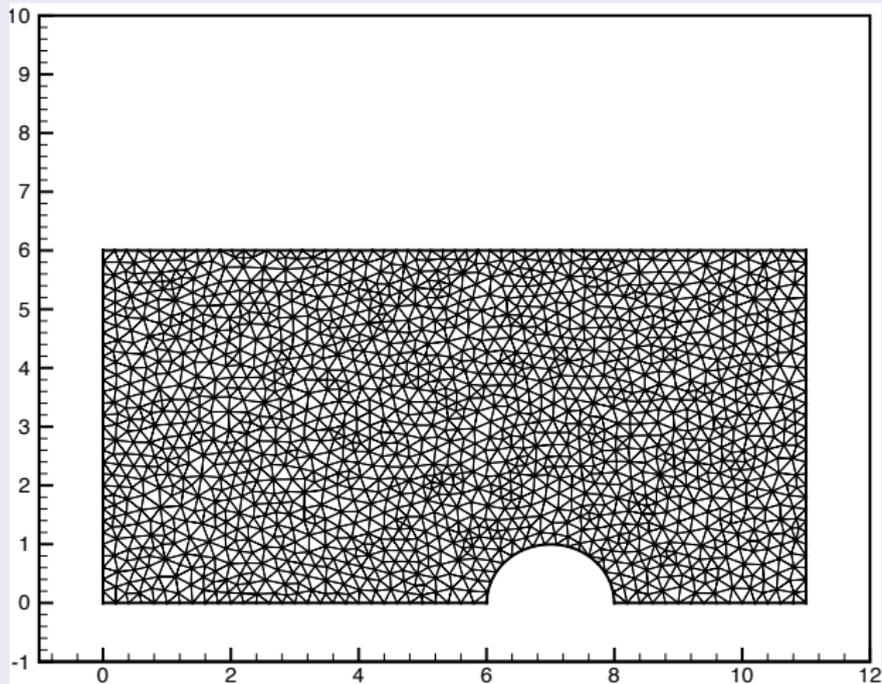


Figure: Initial mesh

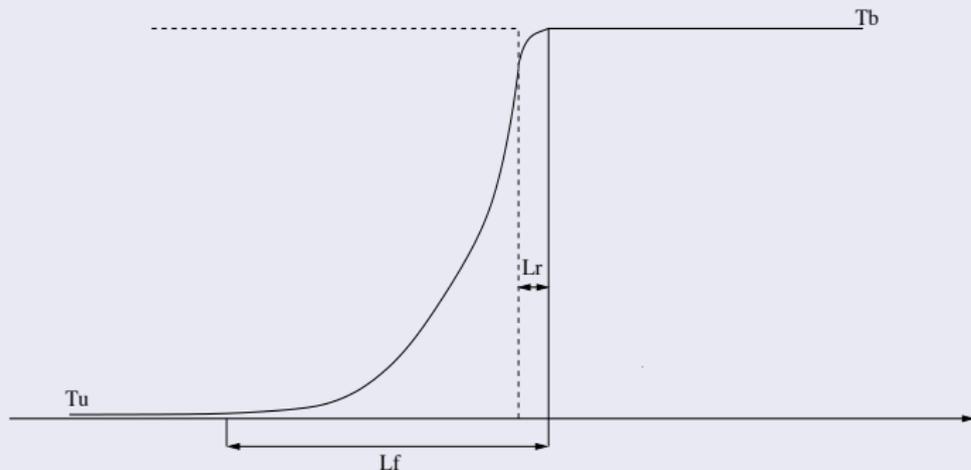
Adaptive Mesh Refinement

High degree of stiffness due to the very different space and time scales;

Thinness of the reaction zone;

Mesh adaptation method is needed during the calculation;

Adaptive procedure based on multi-level refinement and unrefinement,



Adaptive Mesh Refinement

Algorithm based upon a multi level hierarchical tree data structure;
Following the local values of some criterion on macro-element K ,
an integer array called $IADIV$ is updated;
At time $t^n = n\Delta t$, $IADIV(K) = m$ means that K has to be divided
into 4^m triangles.

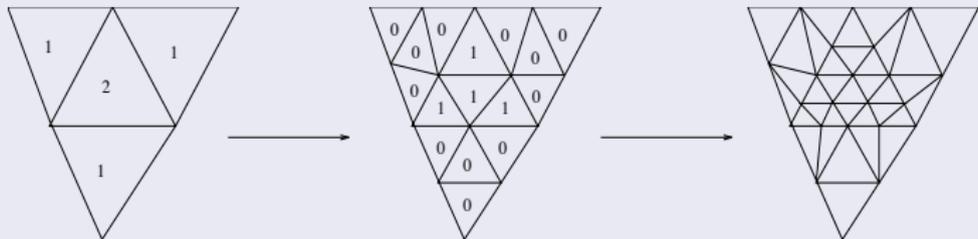


Figure: Refinement process

Simulation Results

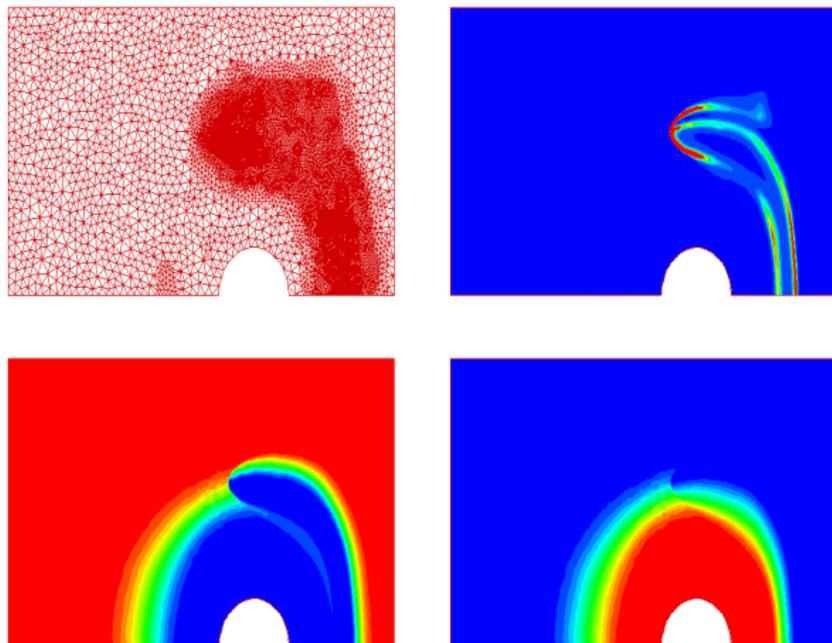


Figure: From left to right and top to bottom: Adaptive mesh, Reaction rate, Oxygen and Fuel

Reaction rate isovalues evolution

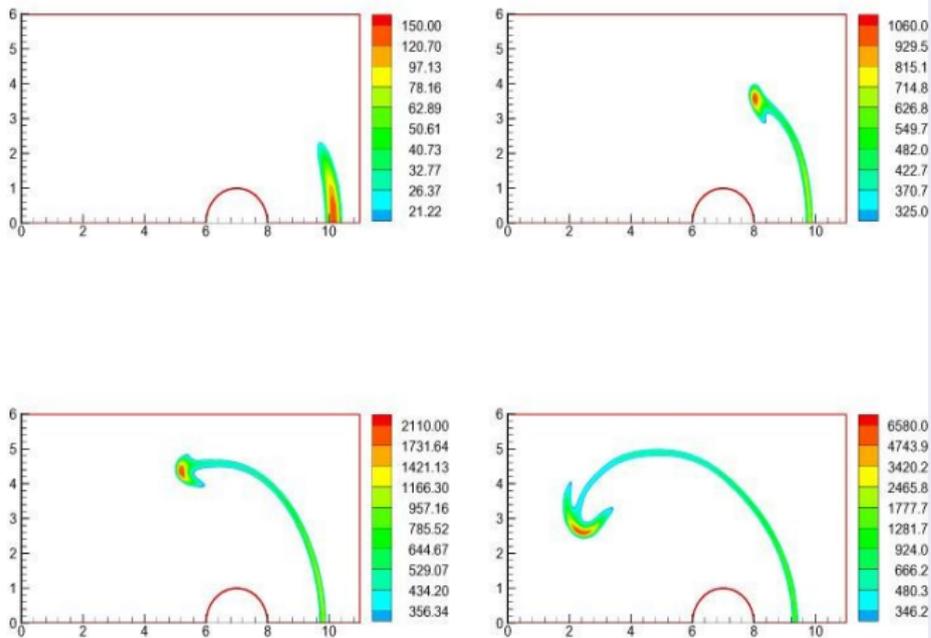
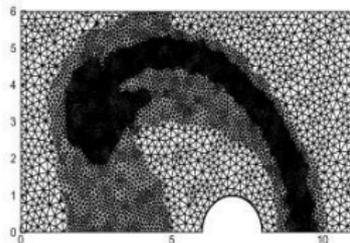
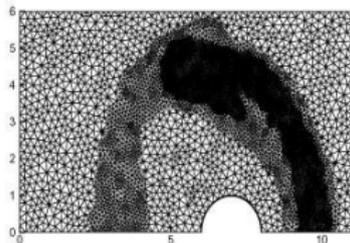
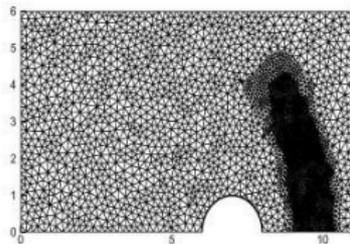
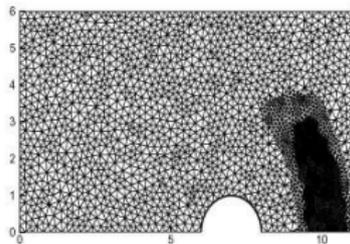


Figure 7: Non-dimensional reaction rate isolines of the mixture at times

Adaptive mesh



The numerical study gave relevant results for the study of droplets ignition in a spray;

It could be shown that the ignition of droplets may occur by involving a triple flame propagation, provided that the reactions are fast enough or droplets large enough;

Results have been obtained only because a mesh adaption, allowing refinements and unrefinements, has been successfully implemented;

The Diamond GreenGauss type interpolation used for the approximation of the diffusion is also found to be determinant

Publications



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PROPAGATION OF STREAMER DISCHARGE IN COLD PLASMA

in collaboration with
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Hot plasma: Nuclear fusion

Nuclear energy:

Fission: breaking up heavier nuclei into lighter, more stable ones;

Fusion: combining elements to form heavier ones;

Sunrise example: fusion of hydrogen to helium using deuterium;

Fusion: Necessity to confine plasma long enough;

The confinement is achieved by using magnetic fields in tokamaks.

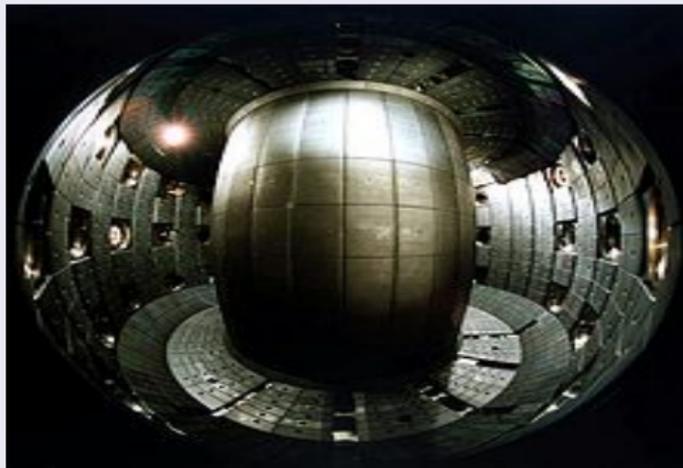


Figure: Tokamak view

Temperatures required for fusion: Destruction of any material that comes into contact with the plasma;

The next generation of tokamak, ITER, is presently under construction in France and it is expected that first plasma operation will occur in 2018.

Tokamak Scheme

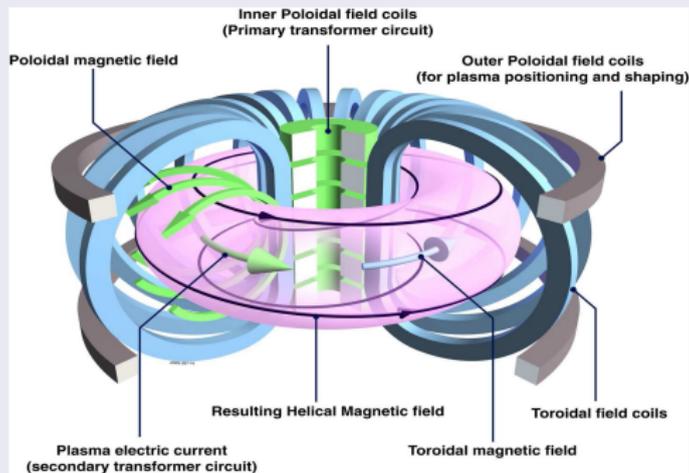


Figure: Schematic view of a Tokamak

Challenges before energy generation from fusion can be a reality;
Study of short events generating large heat loads and vessel forces;
A disruption in a tokamak is an uncontrolled loss of confinement;
Damaging effect on tokamak components;
Loss of confinement: Both thermal and magnetic energy loss.

Cold Plasma: treatment of gas pollution in catalytic muffler

Streamer interest:

Removal of NO_x gas at atmospheric pressure;

Selective technique: producing high energy electrons without heating the gas;

High electrons energy: excitation, dissociation and ionization of the gas;

Give chemically active species and hence decomposition of the pollutant;

Future European environmental standards (NO_x emissions must be reduced from 180 to 80 mg / km in 2014) with reasonable cost

Streamer experiment: Electric circuit

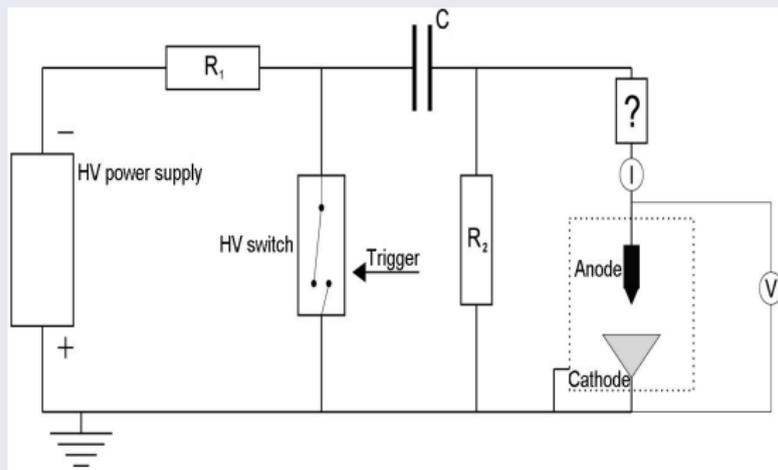


Figure: Electric circuit for pulses up to 30 kV.

Positive streamers in air at 17.5 kV, in a point-plane geometry

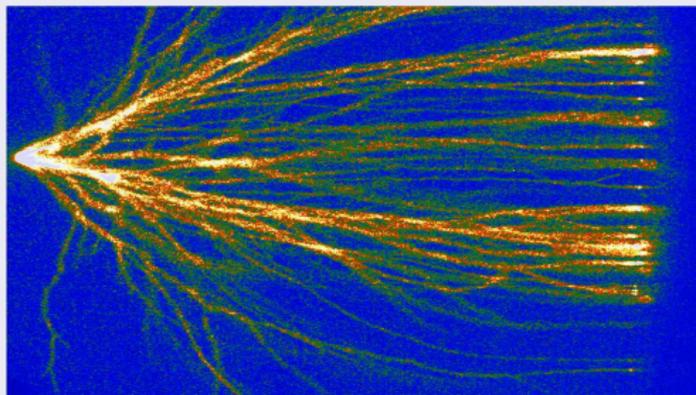


Figure: Positive streamers with a gap of 25 mm shows 70 branches

Evolution of an anode directed streamer in a strong homogeneous background field of 100 kV/cm

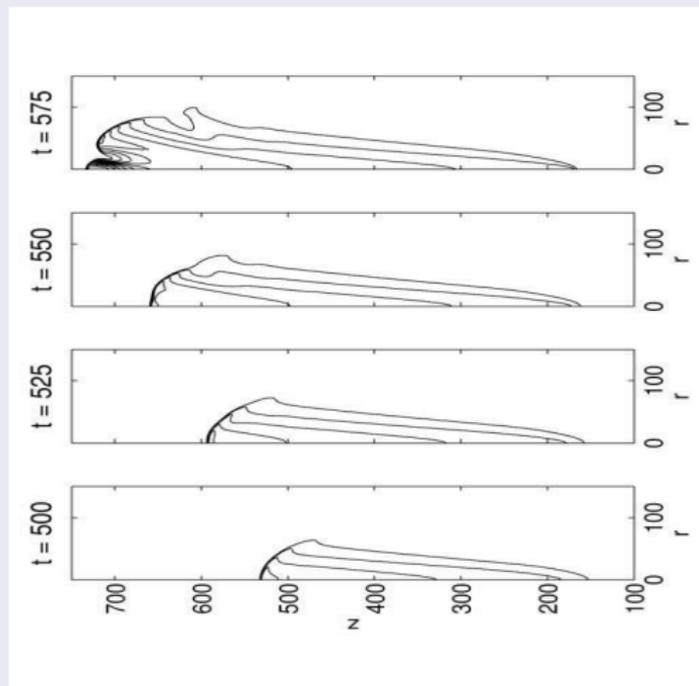


Figure: Levels of equal electron density e_n (Streamer size 4.6 mm).

Cold Plasma: streamer discharges for flame ignition

Transient plasmas: initiation of combustion in propulsion systems and combustion engines;

Corona discharges: overcome the limitations of conventional electric discharges and laser discharge since:

- (1) Many streamers with similar energy content, as opposed to a single, unnecessarily large and intense arc;
- (2) Can initiate combustion in a larger volume,
- (3) the size and shape of the ignition volume can be tailored using the geometry of the anode and cathode.

With recent advances in pulsed power electronics, such discharges can be produced with very high efficiencies in a system of reasonable cost, size and weight.

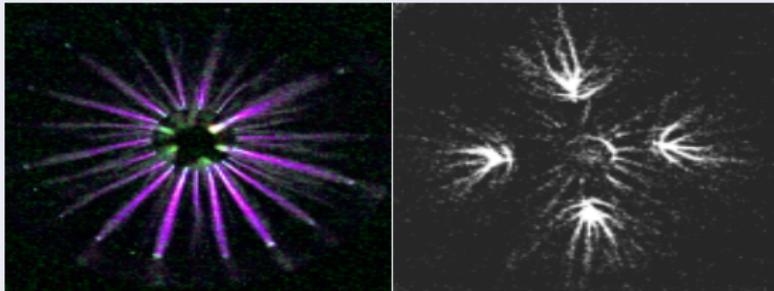


Figure: Images of corona discharges with plain rod electrode. left: axial view of corona discharge using smooth disk attached to electrode to concentrate discharge at one axial location; right: axial view with 4-needles attached to electrode to concentrate discharge at one axial location and 4 azimuthal locations

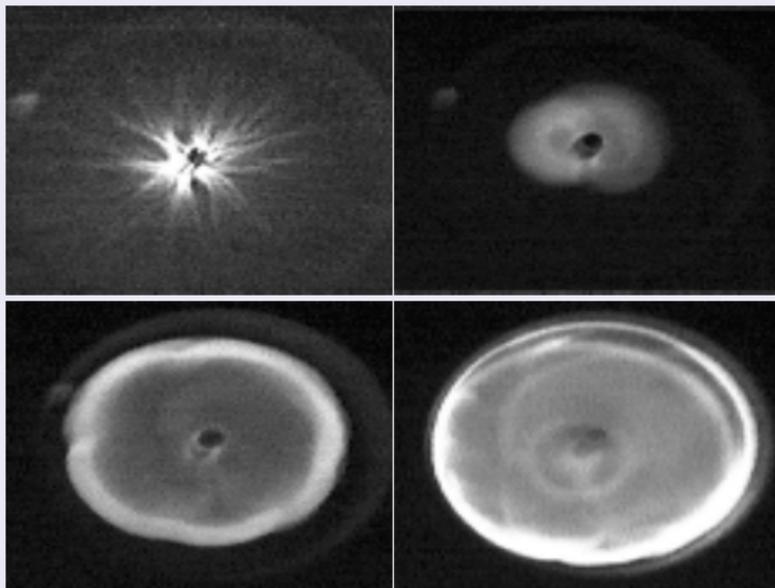


Figure: Sequential photographs (33 ms between images) of axial view of corona discharge ignition of a 6.5% CH₄-air mixture at 1 atm, pulse energy 464 mJ, plain electrode. Chamber diameter is 51 mm.

Numerical simulation of streamer discharge in cold plasma

Considered phenomenon:

Lowly ionized matter exposed to high intensity electric field;

Apparition of a non-equilibrium ionization processes: the discharges;

Various forms depending on the spatio-temporal characteristics of the electric field

One distinguishes the dark, glow or arc discharges such as leaders and streamers;

We've focused on streamers, that are growing filaments of plasma;

Dynamics controlled by highly localized and nonlinear space charge regions.

Basic 2D model of streamer motion;

Convection - diffusion equation for electrons;

simplified equation for ions;

Poissons equation for electric field potential.

Difficulty:

Coupling of electric field and electron motion;

Stiff source terms;

Very steep gradients of unknowns in region of moving front of streamer.

General form of streamer equation

The general form of the streamer equations writes:

$$\frac{\partial n_e}{\partial t} + \operatorname{div}(n_e \vec{v}_e - De \vec{\nabla} n_e) = S_e,$$

$$\frac{\partial n_i}{\partial t} = S_e,$$

$$\Delta V = k \cdot (n_e - n_i),$$

n_e - electron density;
 n_i - ion density;
 v_e - electron drift velocity;
 De - diffusion coefficient;
 S_e - source term;
 V - electric potential;
 $k = \frac{e}{\epsilon_0}$ constant;
 e - elementary charge;
 ϵ_0 - permittivity of vacuum;
Closure:

$$\vec{E} = -\text{grad}(V).$$

Electron drift velocity:

$$\begin{aligned} \text{if } \frac{\|\vec{E}\|}{n} > 2 \cdot 10^{-15}, \quad v_e &= - \left[7.4 \cdot 10^{21} \cdot \frac{\|\vec{E}\|}{n} + 7.1 \cdot 10^6 \right] \cdot \frac{\vec{E}}{\|\vec{E}\|}, \\ 10^{-16} < \frac{\|\vec{E}\|}{n} \leq 2 \cdot 10^{-15}, \quad v_e &= - \left[1.03 \cdot 10^{22} \cdot \frac{\|\vec{E}\|}{n} + 1.3 \cdot 10^6 \right] \cdot \frac{\vec{E}}{\|\vec{E}\|}, \\ 2.6 \cdot 10^{-17} < \frac{\|\vec{E}\|}{n} \leq 10^{-16}, \quad v_e &= - \left[7.2973 \cdot 10^{21} \cdot \frac{\|\vec{E}\|}{n} + 1.63 \cdot 10^6 \right] \cdot \frac{\vec{E}}{\|\vec{E}\|}, \\ \frac{\|\vec{E}\|}{n} \leq 2.6 \cdot 10^{-17}, \quad v_e &= - \left[6.87 \cdot 10^{22} \cdot \frac{\|\vec{E}\|}{n} + 3.38 \cdot 10^4 \right] \cdot \frac{\vec{E}}{\|\vec{E}\|}, \end{aligned}$$

Diffusion coefficient:

$$n = 2.5 \cdot 10^{19} \text{ cm}^{-3}.$$

$$D_e = \left[0.3341 \cdot 10^9 \cdot \left(\frac{\|\vec{E}\|}{n} \right)^{0.54069} \right] \cdot \frac{\|\vec{v}_e\|}{\|\vec{E}\|}.$$

$$S_e = \frac{\alpha}{n} \cdot \|\vec{v}_e\| \cdot n_e \cdot n,$$

$$\text{if } \frac{\|\vec{E}\|}{n} > 1.5 \cdot 10^{-15}, \quad \frac{\alpha}{n} = 2 \cdot 10^{-16} \cdot \exp\left(\frac{-7.248 \cdot 10^{-15}}{\|\vec{E}\|/n}\right),$$

$$\text{else, } \frac{\alpha}{n} = 6.619 \cdot 10^{-17} \cdot \exp\left(\frac{-5.593 \cdot 10^{-15}}{\|\vec{E}\|/n}\right).$$

Finite volume method on unstructured triangular adaptive grid;

Upwind scheme for convective term;

Diamond scheme for diffusion term and Poisson's equation ;

UMFPACK solver of the sparse linear equation system.

Simulation Results

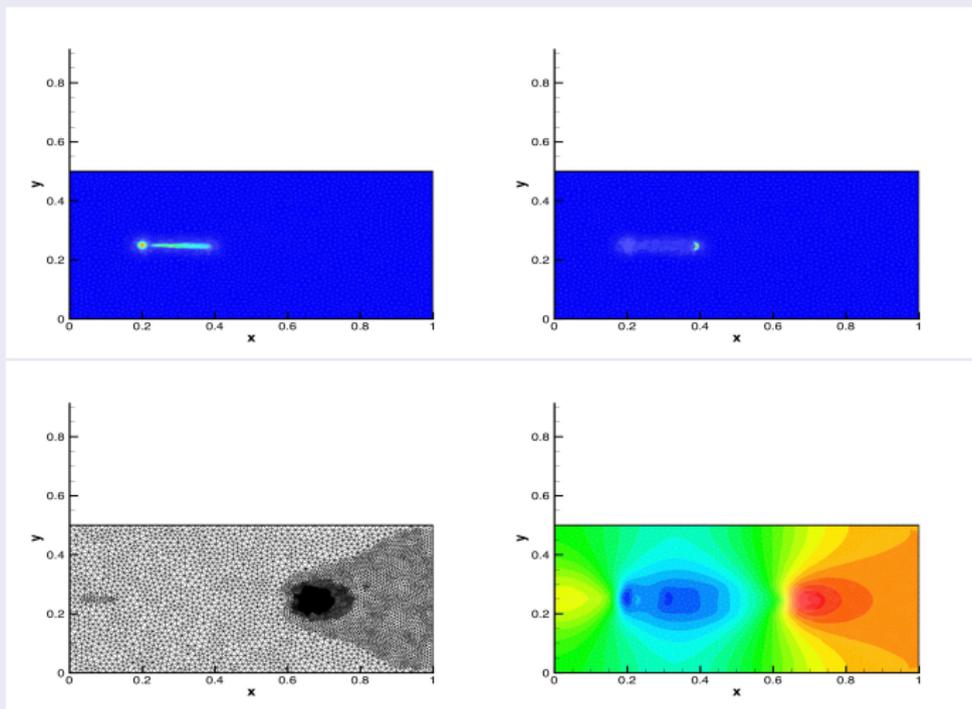


Figure: From left to right and top to bottom: Electron density, source term, adaptive mesh and Electric field

Simulation Results

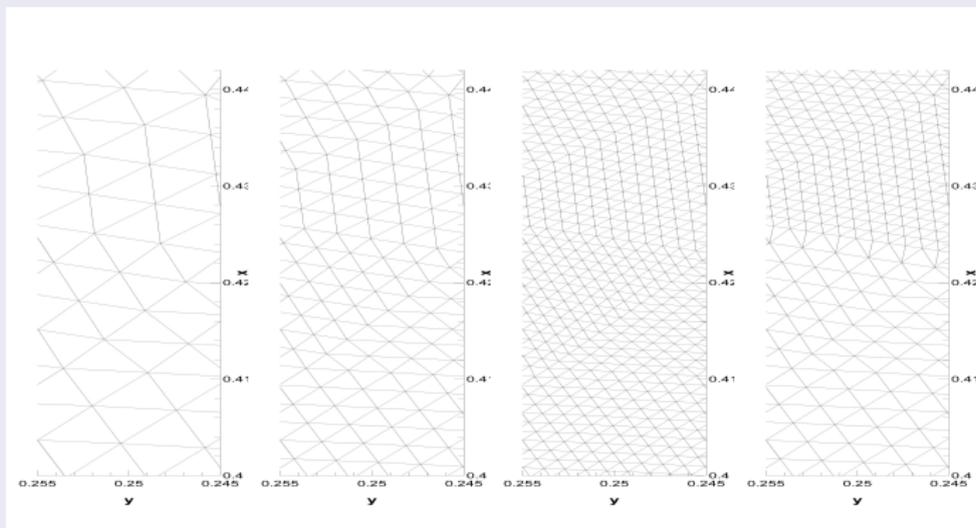


Figure: Fixed mesh with 2, 3, 4 levels of refinement and adaptive mesh

Simulation Results

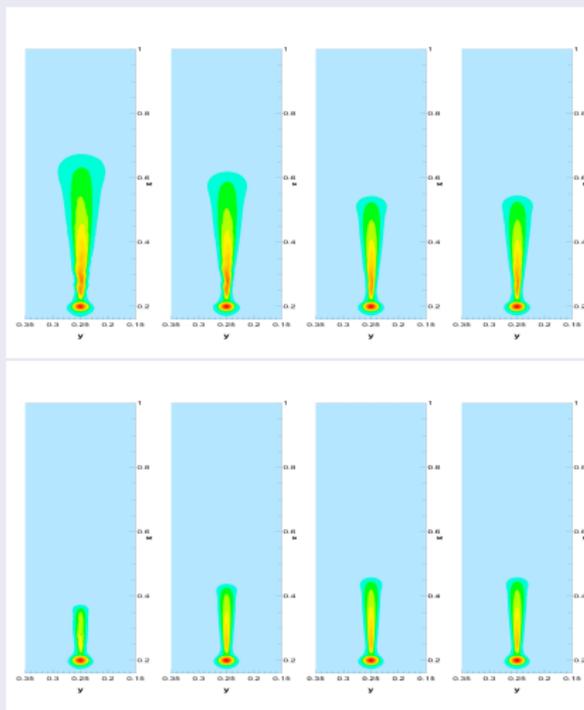


Figure: Electron density. First order (first row), Second order (second row)

Simulation Results

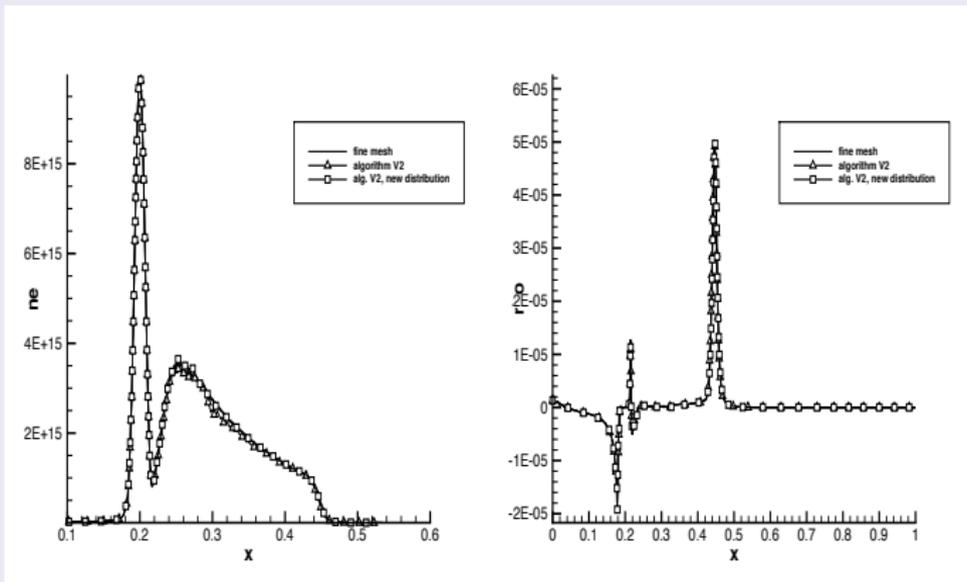


Figure: Second order, comparison of electron density (left) and net charge density (right) computed on fine mesh and mesh with dynamic adaptation

CPU time comparison

	cells	nodes	number of time steps	CPU time
2 levels	75200	37893	2184	1
3 levels	300800	150985	4899	8.158
4 levels	1203200	602769	11222	58.663
adaptation	18636	9392	10845	1.084

Table: CPU time at $t = 5.25 \cdot 10^{-8}s$ using 2^{nd} order precision

Global finite volume method applied to streamer discharge problem;

Accuracy and efficiency of mesh adaptation in 2D framework;

Simplified system of equations;

Ability to capture main problem features;

Localisation of narrow regions with drastic variation of the solution;

Potential for 3D streamer problems in general configuration;

Possible extension to more general plasma problems.

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TRANSPORT IN POROUS MEDIA

in collaboration with Amadou Mahamane⁺ and Mohammed Seaid*

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* Professor at School of Engineering, Durham University, UK

Definition

Porous medium: material containing pores (voids);
Skeletal portion of the material: "matrix" or "frame";
Pores typically filled with fluid (liquid or gas);
Skeletal material: usually a solid;
Foams also often analyzed using concept of porous media.

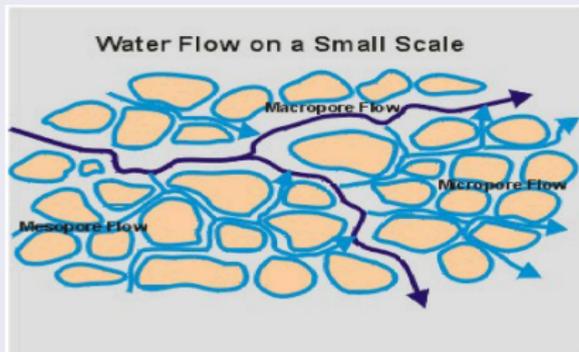


Figure: Flow in porous medium

Porous media: liquid phase in solid pores;

Fundamental in civil engineering and environmental problems:

- * transport of substances,
- * exchanges between solid phases,
- * mechanical stresses by phase changes (crystallization, evaporation);

"Simple" porous media: liquid phase in simple porous solid:
relatively well known;

Porous materials in civil engineering or environment:
generally multi-component, multi-phase and multi-scales.

Oil reservoirs

Key processes in many engineering applications,
Hydrocarbon and geothermal reservoirs;

Wide range of applications:

Reservoir simulation,

CO₂ storage and fundamental flow physics in porous media.

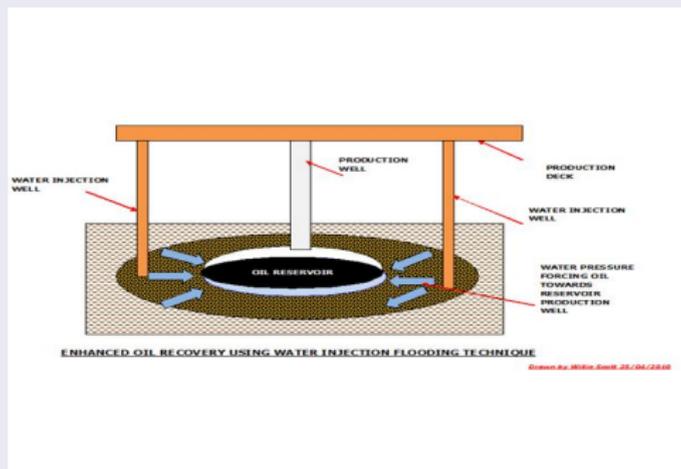


Figure: Reservoir scheme

Transport of dissolved chemical components,
(CO₂, NaCl, CH₄);
Different fluid phases (e.g., water, oil, gas);
Pore spaces in geological formations underground;
Large number of geological and reservoir engineering processes.

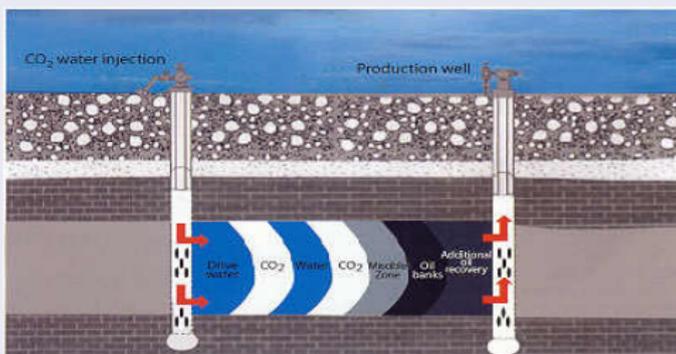


Figure: Enhancing oil recovery and CO₂ storage

Ground water flow

Applications include:

Storing greenhouse gases;

CO₂ in saline aquifers and oil fields;

Enhancing recovery of oil and gas from hydrocarbon reservoirs;

Injection of chemicals or viscosifying polymers;

Flow in the vicinity of radioactive waste repositories;

Remediation of contaminants in groundwater aquifers.

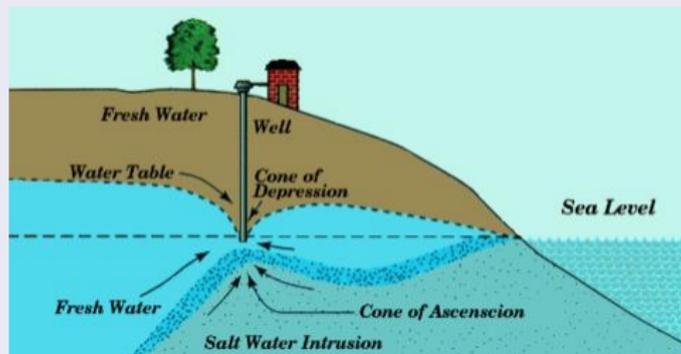


Figure: Fresh and salt water mixing

Flow and transport processes:
Different spatial and temporal scales,
Also local differences;

Highly complex processes in one part of the system:
necessity of fine spatial and temporal resolution;

In other parts of the system, physically simpler processes:
examination on coarser scales.

Considering the porous medium:
Heterogeneous structure,
High dependence on the spatial scale.

Darcy law: simplest and popular law to describe filtration of a fluid in porous medium.

Filtration velocity proportional to difference between body force and pressure gradient.

The governing equations consist of the pressure equation:

$$\mathbf{q} = -d(u)\mathbb{K}(\mathbf{x})\nabla p, \quad (\mathbf{x}, t) \in \Omega \times (0, T],$$

$$\nabla \cdot \mathbf{q} = 0, \quad (\mathbf{x}, t) \in \Omega \times (0, T],$$

$$\mathbf{q} \cdot \mathbf{n}|_{\Gamma_1} = -1.4, \quad \mathbf{q} \cdot \mathbf{n}|_{\Gamma_2} = 0, \quad p|_{\Gamma_3} = 0, \quad t \in (0, T],$$

and the saturation equation

$$\phi(\mathbf{x}) \frac{\partial u}{\partial t} - \nabla \cdot (b(u)\mathbf{q} - \mathbb{K}(\mathbf{x})a(u)\nabla u) = 0, \quad (\mathbf{x}, t) \in \Omega \times (0, T],$$

$$u|_{\Gamma_1} = 1, \quad \mathbb{K} \cdot \mathbf{n}|_{\Gamma_2} = 0, \quad u|_{\Gamma_3} = 0, \quad t \in (0, T],$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega,$$

p : Pressure,

\mathbf{q} : Darcy velocity, u : Saturation,

\mathbb{K} : Permeability of the medium,

ϕ : Porosity

$d(u) = k_w(u) + k_o(u)$: Total mobility.

$$b(u) = \frac{k_w(u)}{k_w(u) + k_o(u)}, \quad a(u) = \frac{k_w(u)k_o(u)}{k_w(u) + k_o(u)} p'(u),$$

$p(u)$: capillary pressure.

The initial condition u_0 is defined as:

$$u_0(\mathbf{x}) = 1 \quad \text{if } \mathbf{x} \in \Gamma_1 \text{ and } 0 \text{ elsewhere}$$

Finite volume method on unstructured triangular adaptive grid;

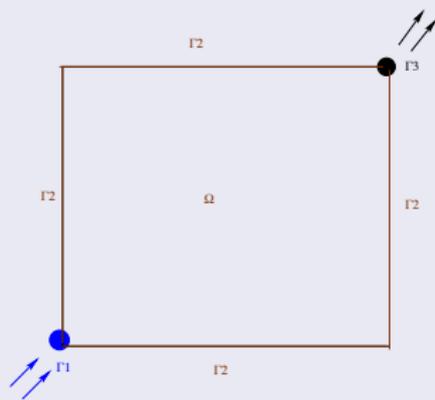
Upwind scheme for convective term;

Diamond scheme for diffusion term and Darcy equation;

GMRES solver of the sparse linear equation system.

Numerical simulation

Ω is a square, $\partial\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$.



Initial & boundary conditions

$$u^0(x) = \begin{cases} 1 & \text{si } x \in \Gamma_1 \\ 0 & \text{si } x \in \Omega \setminus \Gamma_1. \end{cases}$$

$$\mathbf{q} \cdot \mathbf{n}|_{\Gamma_1} = -q_d, \quad \mathbf{q} \cdot \mathbf{n}|_{\Gamma_2} = 0, \quad P|_{\Gamma_3} = 0 \\ u|_{\Gamma_1} = 1, \quad \nabla \alpha(u) \cdot \mathbf{n}|_{\Gamma_2} = 0, \quad u|_{\Gamma_3} = 0$$

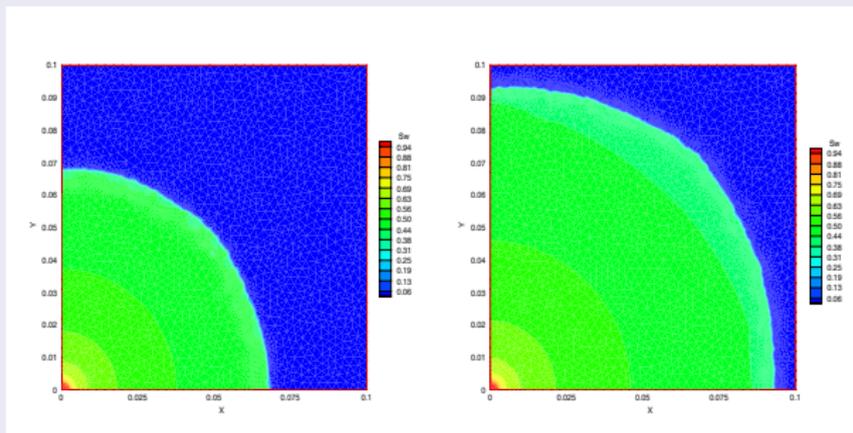
Capilarity and mobility models

$$p_c(u) = -[(1-u)/u]^{\frac{1}{2}}. \\ k_w(u) = \frac{1}{2\mu_w} u^{r_1}, \quad k_o(u) = \frac{(1-u)^{r_2}}{\mu_o}.$$

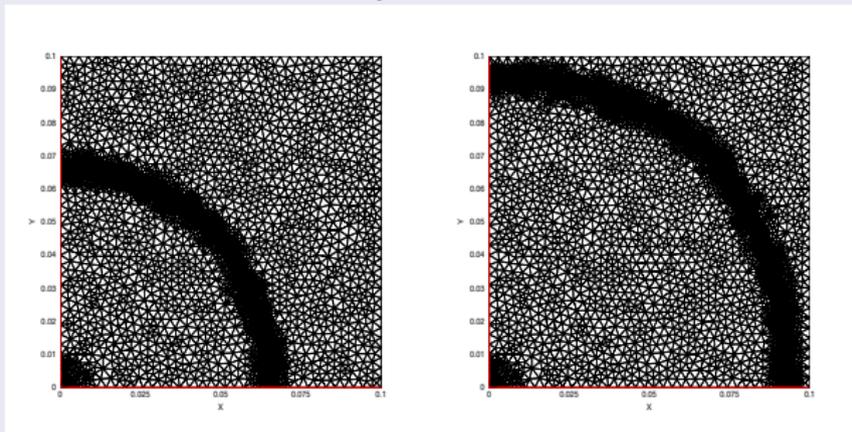
Homogeneous Isotrope Reservoir

$$\Omega =]0, 0.1[^2, \quad q_d = 1.4, \quad \mu_w = 1, \quad \mu_o = 3, \quad r_1 = 5, \quad r_2 = 3$$

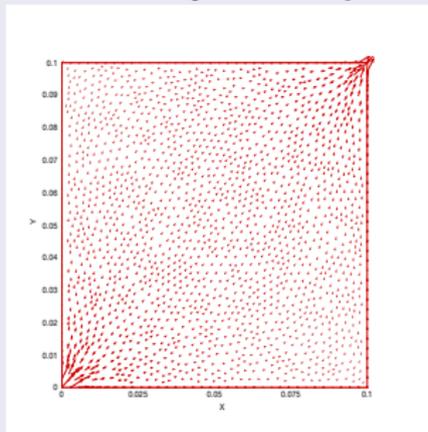
Saturation u



Adaptive mesh



Velociyu field \mathbf{q}

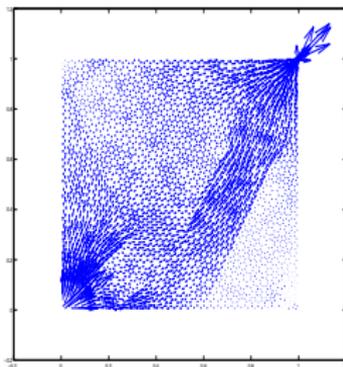
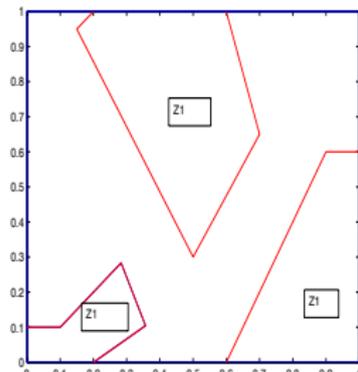


Heterogeneous Reservoir

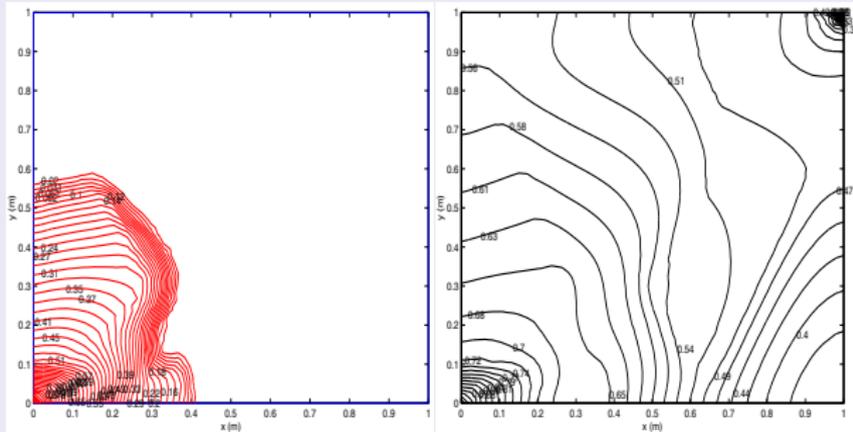
$\Omega =]0, 1[^2$, $q_d = 0.5$, $\mu_w = 1$, $\mu_o = 10$, $r_1 = 3$, $r_2 = 3$

$$\mathbb{K}(\mathbf{x}) = \begin{cases} \begin{bmatrix} 0.1 & 0.03 \\ 0.03 & 0.1 \end{bmatrix} & \text{si } \mathbf{x} \in Z_1 \\ \begin{bmatrix} 1 & 0.3 \\ 0.3 & 1 \end{bmatrix} & \text{si } \mathbf{x} \in \Omega \setminus Z_1 \end{cases}$$

Heterogeneous domain and velocity



Saturation u



Comments and future

Interaction between Darcy pressure and saturation well detected;

Accurate adaptive cell-centered finite volume method;

Significant reduction of the computational cost;

Next step: 3D simulations.



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