Colloque *Une vision transversale des Sciences*
Présentation à l'Institut Henri Poincaré - 22 mai 2018
Ecole Doctorale Galilée, Paris XIII

The DENA Project

Dynamics of MultiScale Expanding Networks

Yves D'Angelo *et al.*

Laboratoire Mathématiques et Interactions J-A Dieudonné
Université Côte d'Azur/Université Nice Sophia Antipolis/CNRS

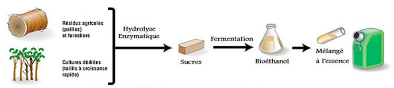
Joint Work with
Laboratoire Interdisciplinaire des Energies de Demain, LIED, Univ. Paris-Diderot
INRIA Sophia-Antipolis
Centre de Mathématiques Appliquées, CMAP, Ecole Polytechnique
Scuola Normale di Pisa, Italy
Università degli Studi di Firenze, Italy
LMO, Laboratoire de Mathématiques d'Orsay.

Synopsis

- **The premises:** ***biology*** *of fungal networks, apexes, hyphae, thallus, mycelium…*
  - ✓ Why studying **Fungi** ?
  - ✓ What is a **mycelium** for ?
  - ✓ **A Multi-Scale** phenomenon…
- **An essential diversion:** *combustion &* ***flames****, reactive flows, active* ***fronts****…*
  - ✓ A **Multi-Scale** phenomenon !
  - ✓ Modeling & High-Performance **Computations**
  - ✓ Simplified modeling, **Evolution** Equations
- **The crux:** *Fungal Propagation*
  - ✓ **A Multi-Scale** phenomenon… : random expanding networks may yield **fronts** !
  - ✓ Tentative **Modeling & Computations**; *Methodology, On-going work, Questions*
  - ✓ An **interdisciplinary** project !
- **The future:** ***Other examples*** *of* ***Expanding*** *(or not)* ***Multi-Scale Networks***

Why studying fungi?

Plant biomass degradation



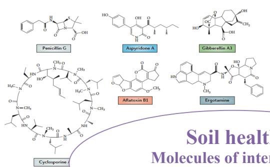
« Bio(Agro)fuel production »

Development of fungal network

Dynamics of expanding complex networks

Since soil carbon is 3 times greater than atmospheric carbon, soil fungi could hugely affect climate change.

Production of seco[…] Metabolites …



Soil health
Molecules of interest in industrial and pharmaceutics areas

[…]ymes

Bioremediation

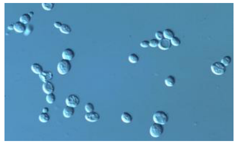
Fungal networks

The present Focus

Characterization of hyphal growth and fungal network

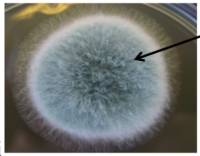
Fungi

Yeasts

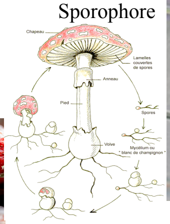



Filamentous fungi

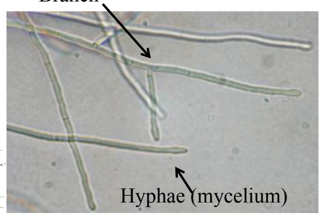
Thallus




Sporophore



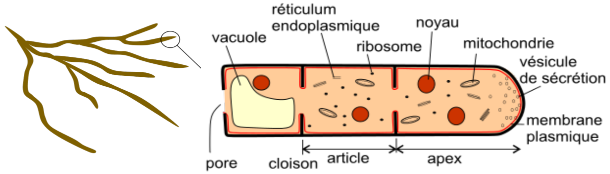
Branch



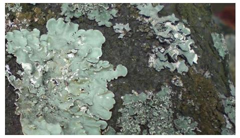
Hyphae (mycelium)

What is a mycelium for?

1/ Nutrition

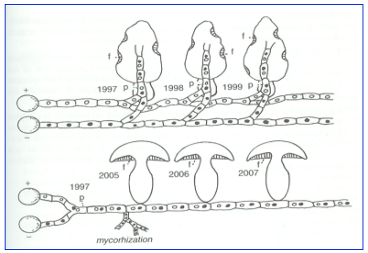


Fungi are *<u>heterotrophic</u>* *and* *<u>absorbotrophic.</u>*
They can live as *<u>saprotrophs, symbiots</u>* *or* *<u>parasites.</u>*

What is a mycelium for?

2/ Reproduction

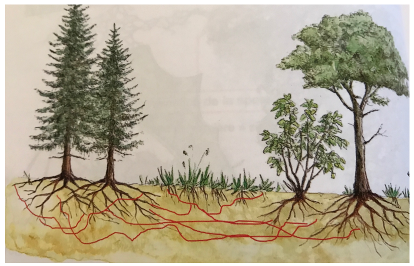


Development of sporophores

« Ronds de sorcières » / « Fairy rings »

What is a mycelium for?

3/ Communication



Mycorrhizae and « underground website »

Ex.: Mycorrhization of Beans (Vicia faba) by Rhizophagus irregularis: chemical communication via the fungal network when Beans are attacked by aphids

(Biodiversité du Monde Fongique, 2015)

What is a mycelium for?

4/ Colonization

Figure 7 - *A cluster of mushrooms at the base of a western white pine. The spores seem to be of limited importance in spreading the fungi.*

Figure 8 - *A cluster of mushrooms on the root of a red oak.*

Figure 10 - *Three disease centers in a virgin, mixed conifer forest in western Montana. The lowermost center covers nearly 20 acres (8 ha).*

(Williams et al., 1989. Forest Insect and Disease)

What is a mycelium for?

4/ Colonization

Ex. Fungal network of *Armillaria ostoyae (solidipes)* in Oregon
8.9 km^2 ; at least 2400 years old; ~ 600 tons

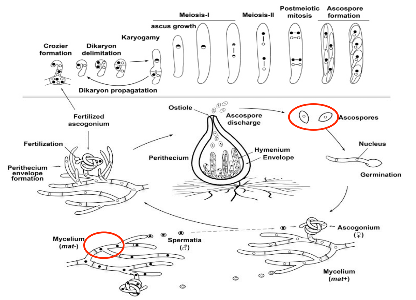
The **hyphal** growth yields a fungal **network,**
able to **adapt** to various constraints ?

- ✓ Physical/chemical constraints: *nutrient deficiency, carbone sources, osmotic and oxydative stresses, temperature, hygrometry, electric field…*
- ✓ Mechanical constraints: *obstacle, labyrinth…*
- ✓ Biological constraints: *other organisms, mutants …*

- ➢ Quantitative analysis of growing hyphae: *speed, hyphae branching*
- ➢ Modeling of fungal network growth

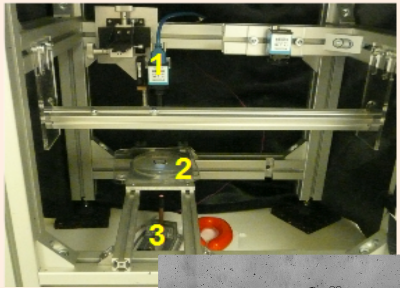
Podospora anserina: a convenient lab model

- ✓ **Ascomycete**
- ✓ **Non pathogenic**
- ✓ **Genome sequenced**
- ✓ **Easy construction of mutants**
- ✓ **Life cycle : 7 days**
- ✓ **Growth in vitro: 27°C – 9 mm/d**

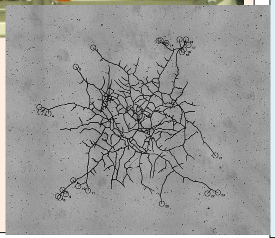


Observation system

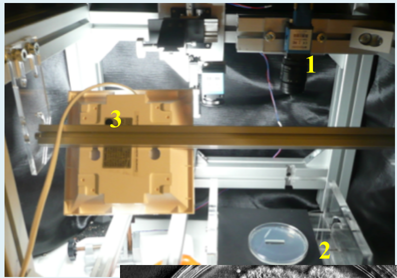
Microscopic observation (× 100)



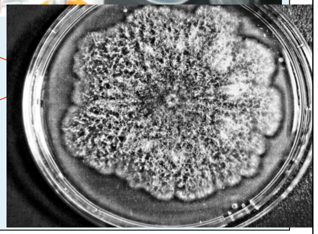
Hyphae



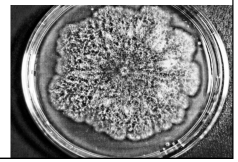
Macroscopic (× 4)



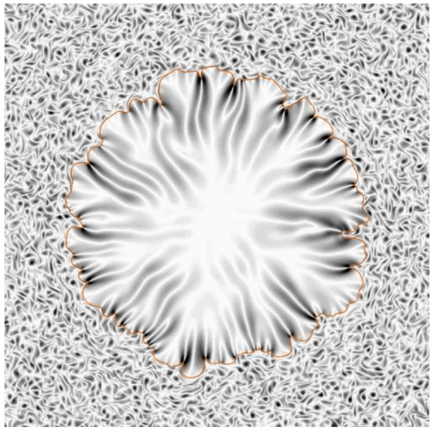
Thallus



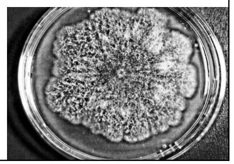
Belousov-Zhabotinsky reaction, in Petri dishes : reaction/diffusion



Flames !!!



Simulation of a 2D methane/air flame in a « turbulent » flow

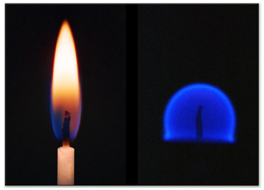


An essential diversion:

combustion & flames, reactive flows, active fronts

- ✓ A Multi-Scale phenomenon !
- ✓ **Modeling** & High-Performance Computations
- ✓ Simplified modeling, Evolution Equations

What is Combustion …?

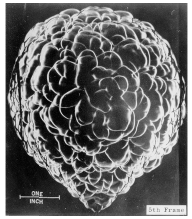


- **Chemical process**, globally irreversible & exothermic, ***coupled*** with
- **Fluid Dynamics**, heat & mass transfer (including radiative transfer)
- *Multiphase Flow…*

Fuel + Air ⟶ CO_2 + H_2O + Other Products + Heat
(including soot, ash and pollutants) (including radiation)

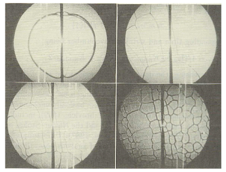
- Heat is released through a very thin zone (the flame front) inducing
  - ✓ high density variations
  - ✓ strong temperature gradients

Pre-mixed flames: Experiments

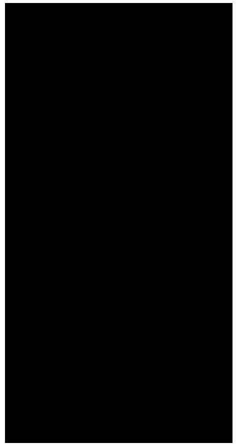


- Propagation of a propane/air flame

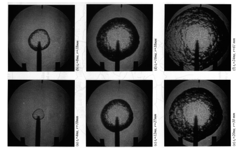
Palm-leis & Strehlow, 1969.



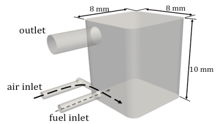
Spark Ignition , Groff, 1982

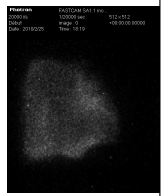


Quinard et al, 2015, IRPHE



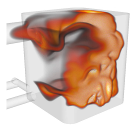
Demoulin CORIA 1999
Front propagation in spray mixtures





Liu et al 2010, CORIA MesoChamber
8 x 8 x 10 mm[3]

How to model flames ? Raw, « Full » Modeling: coupled NL/Stiff PDEs



➢ Small-scale equations are known !

compressible, Low-Mach, Turbulence, stiff complex chemistry, complex molecular transport, soot, radiative transfer, acoustics, shock waves, detonation, multiphase, phase change…

$$\partial_t \rho_g + \nabla.(\rho_g \mathbf{u_g}) = 0,$$

$$\partial_t(\rho_g Y_k) + \nabla.(\rho_g Y_k \mathbf{u_g} + \mathfrak{F}_k) = M_k \omega_k, \qquad \mathrm{U}_k = \frac{\mathfrak{F}_k}{\rho_g Y_k}.$$

$$\partial_t(\rho_g \mathbf{u_g}) + \nabla.(\rho_g \mathbf{u_g} \otimes \mathbf{u_g} + \mathcal{P}_g) = \sum_{1\le k\le n_g} \rho_g Y_k \mathbf{b}_k,$$

$$\partial_t(\rho_g e_g) + \nabla.(\rho_g e_g \mathbf{u_g} + \mathbf{q_g}) = -\mathcal{P}_g : \mathbf{D}_g + \sum_{1\le k\le n_g} \mathfrak{F}_k.\mathbf{b}_k,$$

$$\mathcal{P}_g = p\mathbf{I} - (\kappa_v - \tfrac{2}{3}\eta_v)(\nabla.\mathbf{u_g})\,\mathbf{I} - \eta_v(\nabla\mathbf{u_g} + (\nabla\mathbf{u_g})^t),$$

$$\mathfrak{F}_k = -\sum_{1\le l\le n_g} C_{kl}\mathbf{d}_l - \rho_g Y_k \theta_k \nabla \log T_g, \qquad 1 \le k \le n_g,$$

$$\mathbf{q_g} = \sum_{1\le k\le n_g} h_k \mathfrak{F}_k - \hat{\lambda}\nabla T_g - p\sum_{1\le k\le n_g} \theta_k \mathbf{d}_k.$$

$$\mathbf{d}_k = \nabla X_k + (X_k - Y_k)\nabla \log p + \frac{\rho_g Y_k}{p}\Big(\frac{\sum_{1\le l\le n_g}\rho_g Y_l \mathbf{b}_l}{\sum_{1\le l\le n_g}\rho_g Y_l} - \mathbf{b}_k\Big), \qquad 1 \le k \le n_g,$$

$$\boldsymbol{D}_g = \nabla \mathbf{u_g}.$$

$$e_g = \sum_{1\le k\le n_g} Y_k e_k, \qquad e_k = e_k^{st} + \int_{T^{st}}^{T} c_{vk}(T')\,dT',$$

$$\sum_{1\le k\le n_g} \nu_{ki}^f \chi_k \rightleftharpoons \sum_{1\le k\le n_g} \nu_{ki}^b \chi_k, \qquad 1 \le i \le r,$$

$$\mathcal{P}_k = \sum_{i\in R}\Big(\nu_{ki}^r K_i^d \prod_{l\in S}\gamma_l^{\nu_{li}^f} + \nu_{ki}^d K_i^r \prod_{l\in S}\gamma_l^{\nu_{li}^r}\Big),$$

$$\omega_k = \mathcal{P}_k - Y_k \widehat{\mathcal{N}}_k, \qquad k \in S,$$

$$\mathcal{N}_k = \sum_{i\in R}\Big(\nu_{ki}^d K_i^d \prod_{l\in S}\gamma_l^{\nu_{li}^f} + \nu_{ki}^r K_i^r \prod_{l\in S}\gamma_l^{\nu_{li}^r}\Big).$$

Propane-Air Reaction Mechanism Rate Coefficients in the Form $k_f = AT^\beta \exp(-E/$
Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
1.	$O_2 + H \rightleftharpoons OH + O$	2.000E14	0.0	16820.
2.	$H_2 + O \rightleftharpoons OH + H$	5.060E04	2.67	6290.
3.	$H_2 + OH \rightleftharpoons H_2O + H$	1.000E08	1.6	3300.
4.	$OH + OH \rightleftharpoons H_2O + O$	1.500E09	1.14	100.
5.	$H + H + M' \rightleftharpoons H_2 + M'$	1.800E18	-1.0	0.
6.	$H + OH + M' \rightleftharpoons H_2O + M'$	2.200E22	-2.0	0.
7.	$O + O + M' \rightleftharpoons O_2 + M'$	2.900E17	-1.0	0.
8.	$H + O_2 + M' \rightleftharpoons HO_2 + M'$	2.300E18	-0.8	0.
9.	$HO_2 + H \rightleftharpoons OH + OH$	1.500E14	0.0	1000.
10.	$HO_2 + H \rightleftharpoons H_2 + O_2$	2.500E13	0.0	690.
11.	$HO_2 + H \rightleftharpoons H_2O + O$	3.000E13	0.0	1720.
12.	$HO_2 + O \rightleftharpoons OH + O_2$	1.800E13	0.0	-400.
13.	$HO_2 + OH \rightleftharpoons H_2O + O_2$	6.000E13	0.0	0.
14.	$HO_2 + HO_2 \rightharpoonup H_2O_2 + O_2$	2.500E11	0.0	-1240.
15.	$OH + OH + M' \rightleftharpoons H_2O_2 + M'$	3.256E22	-2.0	0.
16.	$H_2O_2 + H \rightleftharpoons H_2 + HO_2$	1.700E12	0.0	3750.
17.	$H_2O_2 + H \rightleftharpoons H_2O + OH$	1.000E13	0.0	3590.
18.	$H_2O_2 + O \rightleftharpoons OH + HO_2$	2.800E13	0.0	6410.
19.	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$	5.400E12	0.0	1000.
20.	$CO + OH \rightleftharpoons CO_2 + H$	4.400E06	1.5	-740.
21.	$CO + HO_2 \rightleftharpoons CO_2 + OH$	1.500E14	0.0	23610.
22.	$CO + O + M' \rightleftharpoons CO_2 + M'$	7.100E13	0.0	-4545.
23.	$CO + O_2 \rightleftharpoons CO_2 + O$	2.500E12	0.0	47850.
24.	$CH + O \rightleftharpoons CO + H$	4.000E13	0.0	0.
25.	$CH + O_2 \rightleftharpoons CHO + O$	3.000E13	0.0	0.
26.	$CH + CO_2 \rightharpoonup CHO + CO$	3.400E12	0.0	690.
27.	$CHO + H \rightleftharpoons CO + H_2$	2.000E14	0.0	0.
28.	$CHO + O \rightleftharpoons CO + OH$	3.000E13	0.0	0.
29.	$CHO + O \rightleftharpoons CO_2 + H$	3.000E13	0.0	0.
30.	$CHO + OH \rightleftharpoons CO + H_2O$	1.000E14	0.0	0.
31.	$CHO + O_2 \rightleftharpoons CO + HO_2$	3.000E12	0.0	0.
32.	$CHO + M' \rightleftharpoons CO + H + M'$	7.100E14	0.0	16820.

Species for a Propane-Air Flame

C_3H_8	$N*C_3H_7$	$I*C_3H_7$	C_3H_6	C_2H_6	C_2H_5
CH_3CHO	C_2H_4	CH_3CO	C_2H_3	CH_2CO	C_2H_2
C_2HO	C_2H	CH_4	CH_3	CH_2O	CH_2
CHO	CH	CO_2	CO	H_2O_2	H_2O
H_2	HO_2	OH	H	O_2	O
N_2	NO	N			

TABLE II (continued)

Propane-Air Reaction Mechanism Rate Coefficients in the Form $k_f = AT^\beta \exp(-E/RT)$.
Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
33.	$CH_2 + H \rightleftharpoons CH + H_2$	4.000E13	0.0	0.
34.	$CH_2 + O \rightharpoonup CO + H + H$	8.000E13	0.0	0.
35.	$CH_2 + O_2 \rightharpoonup CO + OH + H$	6.500E12	0.0	1500.
36.	$CH_2 + O_2 \rightharpoonup CO_2 + H + H$	6.500E12	0.0	1500.
37.	$CH_2O + H \rightleftharpoons CHO + H_2$	2.500E13	0.0	4000.
38.	$CH_2O + O \rightleftharpoons CHO + OH$	3.500E13	0.0	3490.
39.	$CH_2O + OH \rightleftharpoons CHO + H_2O$	3.000E13	0.0	1200.
40.	$CH_2O + HO_2 \rightleftharpoons CHO + H_2O_2$	1.000E12	0.0	8000.
41.	$CH_2O + CH_3 \rightleftharpoons CHO + CH_4$	1.000E11	0.0	6100.
42.	$CH_2O + M' \rightleftharpoons CHO + H + M'$	1.400E17	0.0	76550.
43.	$CH_3 + H \rightleftharpoons CH_2 + H_2$	1.800E14	0.0	15070.
44.	$CH_3 + O \rightleftharpoons CH_2O + H$	7.000E13	0.0	0.
45.	$CH_3 + OH \rightharpoonup CH_2O + H + H$	9.000E14	0.0	15500.
46.	$CH_3 + OH \rightharpoonup CH_2O + H_2$	8.000E12	0.0	0.
47.	$CH_3 + O_2 \rightharpoonup CH_2O + H + O$	1.500E13	0.0	28710.
48.	$CH_3 + CH_3 \rightleftharpoons C_2H_6$	7.470E52	-11.9	19190.
49.	$CH_3 + M \rightleftharpoons CH_2 + H + M$	1.000E16	0.0	90910.
50.	$CH_3 + CH_3 \rightharpoonup C_2H_4 + H_2$	1.000E16	0.0	32060.
51.	$CH_3 + CH_2 \rightharpoonup C_2H_4 + H$	4.000E13	0.0	0.
52.	$CH_4 + H \rightleftharpoons H_2 + CH_3$	2.200E04	3.0	8760.
53.	$CH_4 + O \rightleftharpoons OH + CH_3$	1.200E07	2.1	7630.
54	$CH_4 + OH \rightleftharpoons H_2O + CH_3$	1.600E06	2.1	2460.
55.	$CH_4 + HO_2 \rightleftharpoons H_2O_2 + CH_3$	4.000E12	0.0	19425.
56.	$CH_4 \rightleftharpoons CH_3 + H$	3.200E34	-6.0	109450.
57.	$CH_4 + CH_2 \rightleftharpoons CH_3 + CH_3$	1.300E13	0.0	9545.
58.	$CH_4 + CH \rightleftharpoons C_2H_4 + H$	3.000E13	0.0	-400.
59.	$C_2H + O \rightleftharpoons CO + CH$	1.000E13	0.0	0.
60.	$C_2H + H_2 \rightleftharpoons C_2H_2 + H$	1.100E13	0.0	2870.
61.	$C_2H + O_2 \rightleftharpoons C_2HO + O$	5.000E13	0.0	1500.
62.	$C_2HO + H \rightleftharpoons CH_2 + CO$	3.000E13	0.0	0.
63.	$C_2HO + O \rightharpoonup CO + CO + H$	1.000E14	0.0	0.
64.	$C_2H_2 + O \rightleftharpoons CH_2 + CO$	4.100E08	1.5	1700.
65.	$C_2H_2 + O \rightleftharpoons C_2HO + H$	4.300E14	0.0	12130.
66.	$C_2H_2 + OH \rightleftharpoons H_2O + C_2H$	1.000E13	0.0	7000.
67.	$C_2H_2 + M \rightleftharpoons C_2H + H + M$	3.600E16	0.0	106700.

Propane-Air Reaction Mechanism Rate Coefficients in the Form $k_f = AT^\beta \exp(-E/RT)$
Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
68.	$CH_2CO + H \rightleftharpoons CH_3 + CO$	7.000E12	0.0	3000.
69.	$CH_2CO + O \rightleftharpoons CHO + CHO$	1.800E12	0.0	1340.
70.	$CH_2CO + OH \rightleftharpoons CH_2O + CHO$	1.000E13	0.0	0.
71.	$CH_2CO + M' \rightleftharpoons CH_2 + CO + M'$	1.000E16	0.0	59330.
72.	$C_2H_3 + H \rightleftharpoons H_2 + C_2H_2$	2.000E13	0.0	0.
73.	$C_2H_3 + O \rightleftharpoons CH_2CO + H$	3.000E13	0.0	0.
74.	$C_2H_3 + O_2 \rightarrow CH_2O + CHO$	1.500E12	0.0	0.
75.	$C_2H_3 \rightleftharpoons C_2H_2 + H$	1.600E32	-5.5	46290.
76.	$CH_3CO + H \rightleftharpoons CH_2CO + H_2$	2.000E13	0.0	0.
77.	$CH_3CO + O \rightleftharpoons CH_3 + CO_2$	2.000E13	0.0	0.
78.	$CH_3CO + CH_3 \rightleftharpoons C_2H_6 + CO$	5.000E13	0.0	0.
79.	$CH_3CO \rightleftharpoons CH_3 + CO$	2.300E26	-5.0	17990.
80.	$C_2H_4 + H \rightleftharpoons C_2H_3 + H_2$	1.500E14	0.0	10215.
81.	$C_2H_4 + O \rightarrow CH_3CO + H$	1.600E09	1.2	740.
82.	$C_2H_4 + OH \rightleftharpoons C_2H_3 + H_2O$	3.000E13	0.0	3000.
83.	$C_2H_4 + CH_3 \rightleftharpoons C_2H_3 + CH_4$	4.200E11	0.0	11120.
84.	$C_2H_4 + M' \rightleftharpoons C_2H_2 + H_2 + M'$	2.500E17	0.0	76500.
85.	$CH_3CHO + H \rightleftharpoons CH_3CO + H_2$	4.000E13	0.0	4210.
86.	$CH_3CHO + O \rightleftharpoons CH_3CO + OH$	5.000E12	0.0	1790.
87.	$CH_3CHO + OH \rightleftharpoons CH_3CO + H_2O$	8.000E12	0.0	0.
88.	$CH_3CHO + HO_2 \rightleftharpoons CH_3CO + H_2O_2$	1.700E12	0.0	10720.
89.	$CH_3CHO + CH_2 \rightleftharpoons CH_3CO + CH_3$	2.500E12	0.0	3800.
90.	$CH_3CHO + CH_3 \rightleftharpoons CH_3CO + CH_4$	8.500E10	0.0	6000.
91.	$CH_3CHO \rightleftharpoons CH_3 + CHO$	2.000E15	0.0	79190.
92.	$C_2H_5 + H \rightleftharpoons CH_3 + CH_3$	3.000E13	0.0	0.
93.	$C_2H_5 + O \rightleftharpoons CH_3CHO + H$	5.000E13	0.0	0.
94.	$C_2H_5 + O_2 \rightleftharpoons HO_2 + C_2H_4$	2.000E12	0.0	5000.
95.	$C_2H_5 + CH_3 \rightleftharpoons C_3H_8$	7.000E12	0.0	0.
96.	$C_2H_5 + C_2H_5 \rightleftharpoons C_2H_4 + C_2H_6$	1.400E12	0.0	0.
97.	$C_2H_5 \rightleftharpoons C_2H_4 + H$	1.300E19	-2.0	41480.
98.	$C_2H_6 + H \rightleftharpoons H_2 + C_2H_5$	5.400E02	3.5	5215.
99.	$C_2H_6 + O \rightleftharpoons OH + C_2H_5$	3.000E07	2.0	5120.
100.	$C_2H_6 + OH \rightleftharpoons H_2O + C_2H_5$	6.300E06	2.0	645.
101.	$C_2H_6 + HO_2 \rightleftharpoons H_2O_2 + C_2H_5$	6.000E12	0.0	19420.
102.	$C_2H_6 + CH_3 \rightleftharpoons C_2H_5 + CH_4$	5.500E-01	4.0	8300.
103.	$C_2H_6 + CH_2 \rightleftharpoons CH_3 + C_2H_5$	2.200E13	0.0	8680.
104.	$C_2H_6 + CH \rightleftharpoons H + C_3H_6$	1.100E14	0.0	-260.

Propane-Air Reaction Mechanism Rate Coefficients in the Form $k_f = AT^\beta \exp(-E/RT)$
Units are moles, cubic centimeters, seconds, Kelvins and calories/mole.

	REACTION	A	β	E
105.	$C_3H_8 + H \rightleftharpoons N*C_3H_7 + H_2$	1.300E14	0.0	9710.
106.	$C_3H_8 + H \rightleftharpoons I*C_3H_7 + H_2$	1.000E14	0.0	8350.
107.	$C_3H_8 + O \rightleftharpoons N*C_3H_7 + OH$	3.000E13	0.0	5765.
108.	$C_3H_8 + O \rightleftharpoons I*C_3H_7 + OH$	2.600E13	0.0	4470.
109.	$C_3H_8 + OH \rightleftharpoons N*C_3H_7 + H_2O$	6.300E06	2.0	645.
110.	$C_3H_8 + OH \rightleftharpoons I*C_3H_7 + H_2O$	1.200E08	1.46	-190.
111.	$C_3H_8 + HO_2 \rightleftharpoons N*C_3H_7 + H_2O_2$	6.000E12	0.0	19420.
112.	$C_3H_8 + HO_2 \rightleftharpoons I*C_3H_7 + H_2O_2$	2.000E12	0.0	17000.
113.	$C_3H_8 + CH_3 \rightleftharpoons N*C_3H_7 + CH_4$	7.500E12	0.0	14950.
114.	$C_3H_8 + CH_3 \rightleftharpoons I*C_3H_7 + CH_4$	4.300E12	0.0	13280.
115.	$N*C_3H_7 + H \rightleftharpoons C_3H_8$	2.000E13	0.0	0.
116.	$I*C_3H_7 + H \rightleftharpoons C_3H_8$	2.000E13	0.0	0.
117.	$N*C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	1.000E12	0.0	5000.
118.	$I*C_3H_7 + O_2 \rightleftharpoons C_3H_6 + HO_2$	1.000E12	0.0	2990.
119.	$N*C_3H_7 \rightleftharpoons C_3H_6 + H$	1.000E14	0.0	37340.
120.	$I*C_3H_7 \rightleftharpoons C_3H_6 + H$	2.000E14	0.0	38730.
121.	$N*C_3H_7 \rightleftharpoons C_2H_4 + CH_3$	3.000E14	0.0	33250.
122.	$C_3H_6 + O \rightleftharpoons CH_3CO + CH_3$	5.000E12	0.0	450.
123.	$C_3H_6 + OH \rightarrow C_2H_2 + CH_3 + H_2O$	2.000E13	0.0	3060.
124.	$N_2 + O \rightleftharpoons N + NO$	0.136E15	0.0	76400.
125.	$N + O_2 \rightleftharpoons O + NO$	0.267E11	0.72	7080.
126.	$N + OH \rightleftharpoons H + NO$	0.280E14	0.0	0.

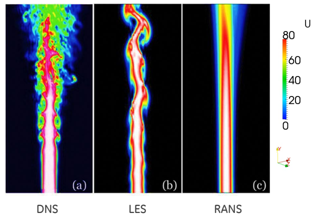
Third body efficiencies for M' : $\alpha(O_2) = 0.4$, $\alpha(N_2) = 0.4$, $\alpha(CO) = 0.75$, $\alpha(CO_2) = 1.5$, $\alpha(H_2O) = 6.5$, $\alpha(C_3H8) = 3$.

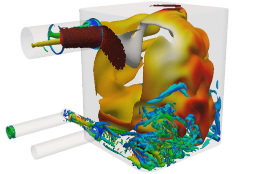
$$\omega_{CO_2}, \omega_{C_3H_8}, \omega_{O_2}, \omega_{H_2O}, \omega_{OH}, \omega_{CH}, \ldots$$

Effective Modeling ?

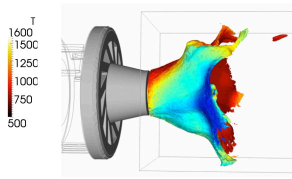
- **RANS, U-RANS, LES, DES, DNS…**

Turbulence + Turbulent Combustion Modeling, Skeletal or Complex Chemistry, Simplified or Complex (molecular) Transport, Sub-Grid Scale Modelling…





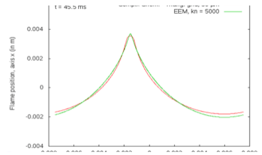
Well resolved LES



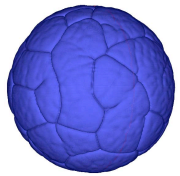
Coarse-Grained LES

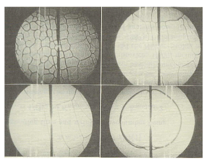
- Thin fronts: equation(s) for the front, **Evolution Equation Modeling**

(e.g. a **perturbative** approach, based **on density contrast asymptotics)**



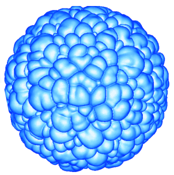
Evolution-Equation Modeling approach

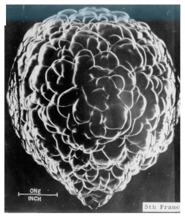




Groff, 1982.

« Soccer-Ball » Flame (cf. Zel'dovich)



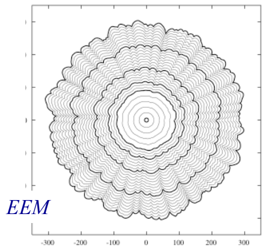


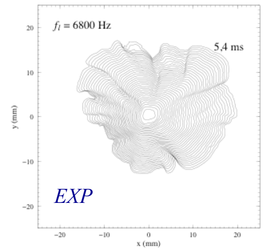
« Cauliflower » flames

$$\frac{\partial F}{\partial t} - \frac{a(\alpha)}{2} S_L \frac{|\nabla_S F|^2}{r_F^2} = \Omega(\alpha) S_L \left(\frac{H(F)}{r_F} - \frac{C(F)}{k_n r_F^2} \right) + CT + u'$$

δ-correlated forcing

Spectral (Fourier-Legendre) resolution in space, coupled with ETDRK schemes in time

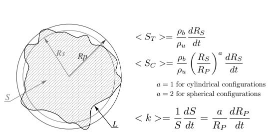


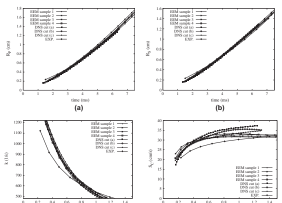


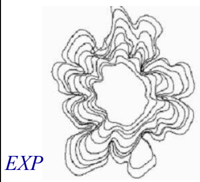
Notice the angular invariance !

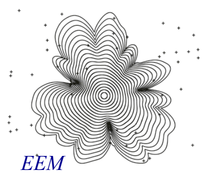
Comparison of 3D EEM results (equatorial cuts) with experiments by Lecordier (1999)

Experimentaly determined Flame Velocities





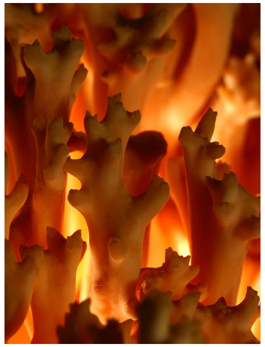




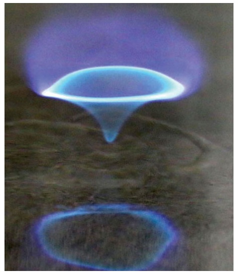
Expanding 2D fronts

Right : with a Dold-Joulin type equation, in a correlated velocity field (the + are the centers of radially elongated Gaussian vortices)

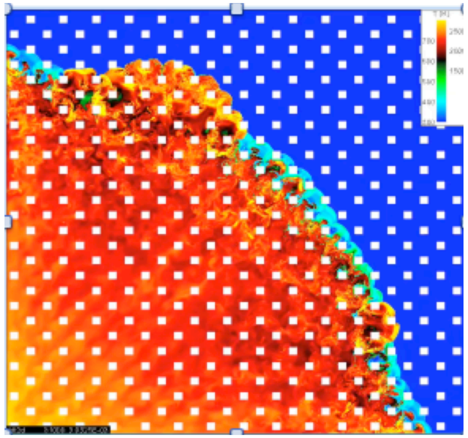
Left : Experimental cuts of an expanding 3D flame (Renou, 2003)



Fungi and Flames ?



Propagating Fronts in Fluid Dynamics



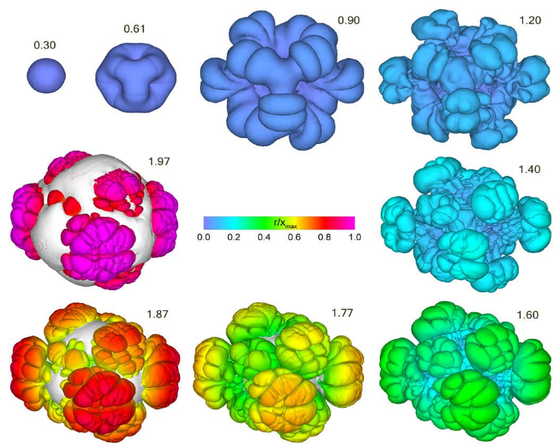
Oran et al.

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla P &= 0, \\
\frac{\partial E}{\partial t} + \nabla \cdot \left((E+P)\mathbf{u}\right) + \nabla \cdot \left(K \nabla T\right) &= \rho q \dot{w}, \\
\frac{\partial \rho Y}{\partial t} + \nabla \cdot \left(\rho Y \mathbf{u}\right) + \nabla \cdot \left(\rho D \nabla Y\right) &= \rho \dot{w}.
\end{aligned}$$

$$\dot{w} = -A \rho Y \exp\left(-\frac{Q}{RT}\right),$$

Pre-mixed Flames, Detonations, Deflagration-to-Detonation Transition

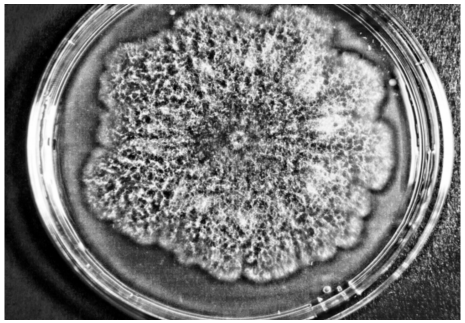
Simulation of a Type Ia Supernova Delayed Detonation



Oran et al.

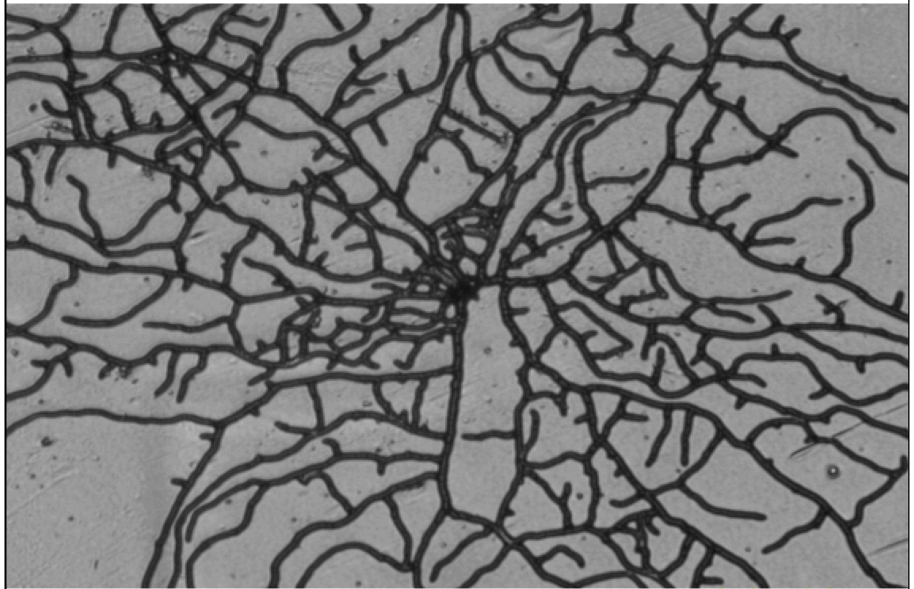
Ia Type Supernovae :« Burning of carbon and oxygen to heavier elements, notably nickel 56 »

Fungal Fronts Propagation

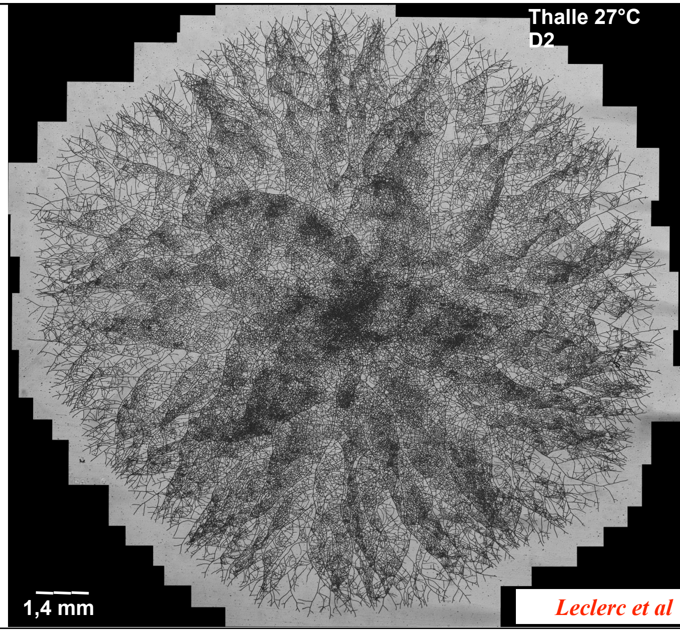


How much does a Thallus Growth resemble (or not) a Flame Propagation ?

Leclerc et al, 2017



Leclerc et al

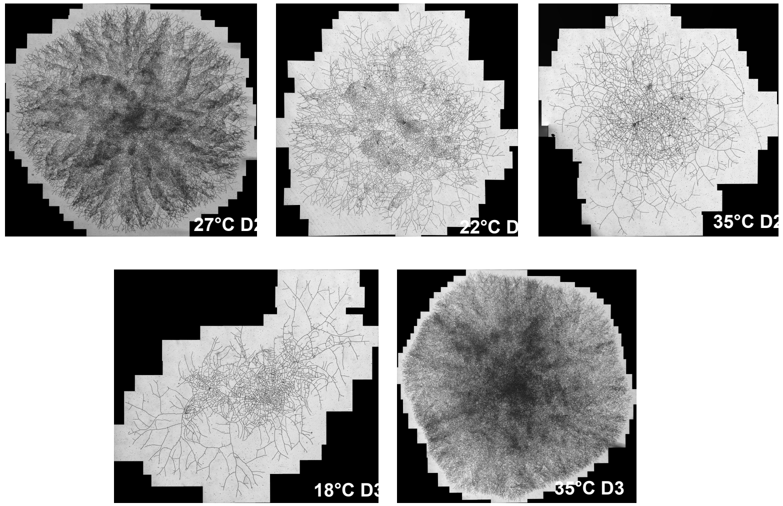


Leclerc et al

Fungal network of *Armillaria ostoyae* *(solidipes)* in Oregon

8.9 km² ; at least 2400 years old; 600 tons

Reconstitution of thallus, under constraints



Leclerc et al

Different levels of descriptions

1 **Microscopic Scale**
Trajectories X_i , V_i of each « particle » (the apex, i.e. the tip of the hypha), including histories

2 **Mesoscopic Scale**
Evolution of $f(X,V,t)$
At time t, the number of particles within $\mathcal{X}$ and with velocity in $\mathcal{V}$ is

$$\int_{\mathcal{X}} \int_{\mathcal{V}} f(X,V,t)\, dX\, dV$$

3 **Macroscopic Scale**
Evolution of observable quantities (concentrations, velocity field, network, number of apexes, …) : *Balance Equations, System of coupled nonlinear PDEs*

4 ***Evolution Equation for the Front itself !***
EEM

Evolution of the Two-Dimensional hyphal network of *P. Anserina*

- Several microscopic features: motion, branching, sub-branching, self-avoidance...
- Aim of the mathematical model
  - ✓ Rigorous description of (some of) the **microscopic** phenomena
  - ✓ **Multi-scale modelling**: from the micro to the mesoscopic scales (then to larger scales)
  - ✓ Mathematical tools at the micro/meso scopic level:

    branching, sub-branching, anastomosis,

    mean-field interacting particles system with memory, coupled with **PDEs**.

Motion

- The apexes are characterized by their **velocity** and **position**
- **Inertial** motion with **friction** …
- … as well as **some randomness**

Mathematically if X^i is the position of the i-th apex, and V^i is its velocity.

$$\begin{cases} \frac{\mathrm{d}X_t^i}{\mathrm{d}t} = V_t^i \\ \frac{\mathrm{d}V_t^i}{\mathrm{d}t} = -\lambda V_t^i + \sigma \frac{\mathrm{d}B_t^i}{\mathrm{d}t} \end{cases}$$

where $(B^i)_{i\in\mathbb{N}}$ is a family of independent Brownian motions.

Motion within a nutrient field

- The apexes evolve in a **nutrient field**: they tend to move towards regions where more nutrient is present.
- The living hyphal network consumes the nutrients, within a **certain distance** around it.
- The nutrient field can be modeled as a (network-coupled) **repulsive potential**
- The apexes (the particles) are **moving** within the potential.

At time $t \in [0,T]$ there are N_t^N particles, "alive" (i.e. moving) or having lived, and the initial value is $N_0^N = N$.
The $i-th$ particle appears at time $T^{i,N}$ and disappears at time $\Theta^{i,N}$.
For $t \in [T^{i,N}, \Theta^{i,N})$, the motion of the $i-th$ particle is driven by the following set of kinetic equations :

$$\begin{cases} \mathrm{d}X_t^{i,N} = V_t^{i,N}\,\mathrm{d}t \\ \mathrm{d}V_t^{i,N} = -\lambda V_t^{i,N}\,\mathrm{d}t + \nabla C^N(t, X_t^{i,N})\,\mathrm{d}t + \sigma\,\mathrm{d}B_t^i \end{cases},$$

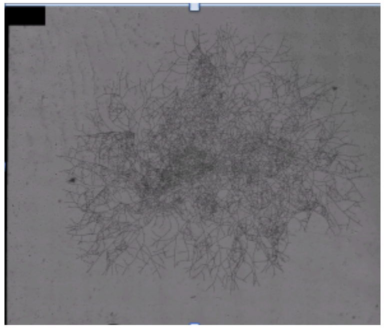
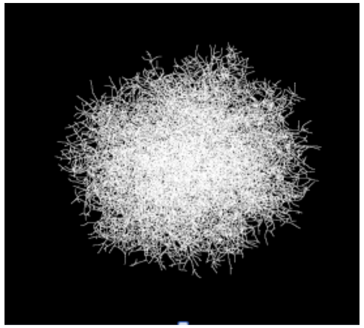
where $\left((B_t^i)_{t\in[0,T]}\right)_{i\in\mathbb{N}}$ is a family of independent standard Brownian motions, λ denotes the friction coefficient, and C^N denotes a potential (nutrient or something else).

Branching within the Tips

- The apexes are the TIPS of the branching network.
- The apexes may branch and give birth to a new (additional) apex.

Creation (sub-branching) and Merging

- An apex can appear along a branch within the living network.
- Conversely, when an apex meets the living network, **anastomosis** may occur.

Ascopore
1cm x 1cm
30h20 experiment duration
20 min between 2 images, 91 images

Ricci et al
(Work in progress)

Statistical Analysis :
Olivier et al
Work in progress…

Dikec, Leclerc et all, Work in progress

Different levels of descriptions

1 **Microscopic Scale**
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2 **Mesoscopic Scale**
Evolution of $f(X,V,t)$
At time t, the number of particles within $\mathcal{X}$ and with velocity in $\mathcal{V}$ is

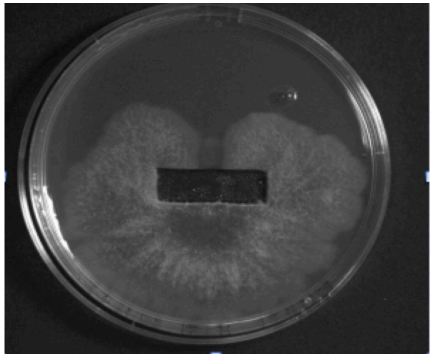
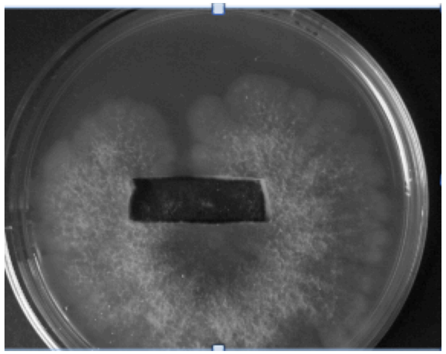
$$\int_{\mathcal{X}} \int_{\mathcal{V}} f(X,V,t) dX dV$$

3 **Macroscopic Scale**
Evolution of observable quantities (concentrations, velocity field, network, number of apexes, …) : *Balance Equations,*
System of coupled nonlinear PDEs

4 *Evolution Equation for the Front itself !*
EEM

1-2-3-4 bis Above Mathematics and Benchmarking,
Numerical analysis and HP computations !!!
As well as Physical/Biological Interpretation

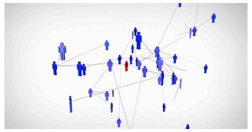
Dynamic observation of thallus growth: presence of an obstacle

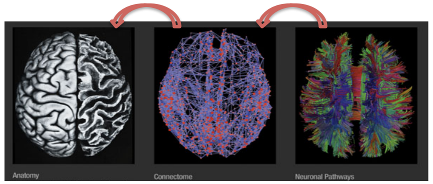
The Thallus DOES NOT behave exactly like a flame…

Leclerc et al
Work in progress

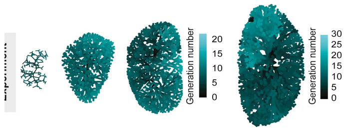
Dynamic Expanding Networks



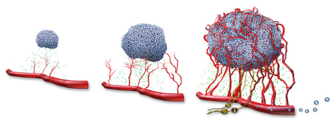
Social networks



Neural networks



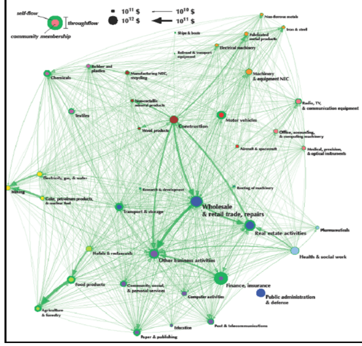
Organ Growth in Mammals (here kidney growth, *Cell, 2017*)



Tumor Growth, anastomosis

Population Dynamics, Epidemiology

The clip depicts the time course of a simulated pandemic with initial outbreak in Atlanta, USA. The panels on the left and right depict the same simulation, only in different representations. On the left one observes a concentric, expanding wave front in the effective distance representation. The same simulation exhibits more complex spatio-temporal structure in the conventional geographic representation on the right. (Brockman et al, science, 2014).



An example of inter-industry network of a national economy. *McNerley et al., Physica D, 2013*

Conclusions, Perspectives

- **Interdisciplinary Project** : **biology, physics, thermodynamics, probabilistic modeling and analysis, statistics, PDEs, control theory, optimization, numerical analysis, scientific computing, HPC…**
- **Multi-scale Analysis: micro, meso, macro, kinetic equations, fronts, EEM…**
- **Many other possible applications, including human health, cancer growth modeling, economy, fake news spreading, neural networks, mammal organs growth…**
- **About 15 people involved in Nice, Paris area, Florence, Pisa…**
- **Hands (and brains) required !**

The DENA Project

LJAD
Rémi Catellier
Laurent Monasse
Thierry Goudon
Yves D'Angelo

Scuola Normale di Pisa
Cristiano Ricci
Franco Flandoli

LIED Paris–Diderot Biology Group
Gwënael Ruprich-Robert
Jonathan Dikec
Hervé Lalucque
Florence Leclerc

LIED Paris–Diderot Physics Group
Cécilia Bobée
Eric Herbert
Christophe Goupil

CMAP Ecole Polytechnique
Jules Depersin
Amandine Véber

LMO Orsay
Adélaïde Olivier

Thanks !