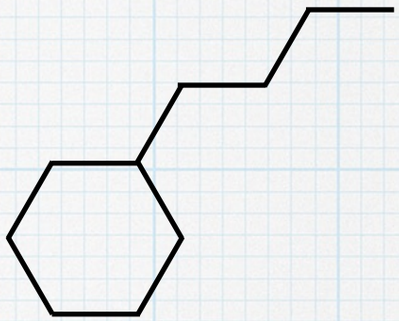
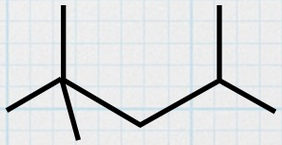


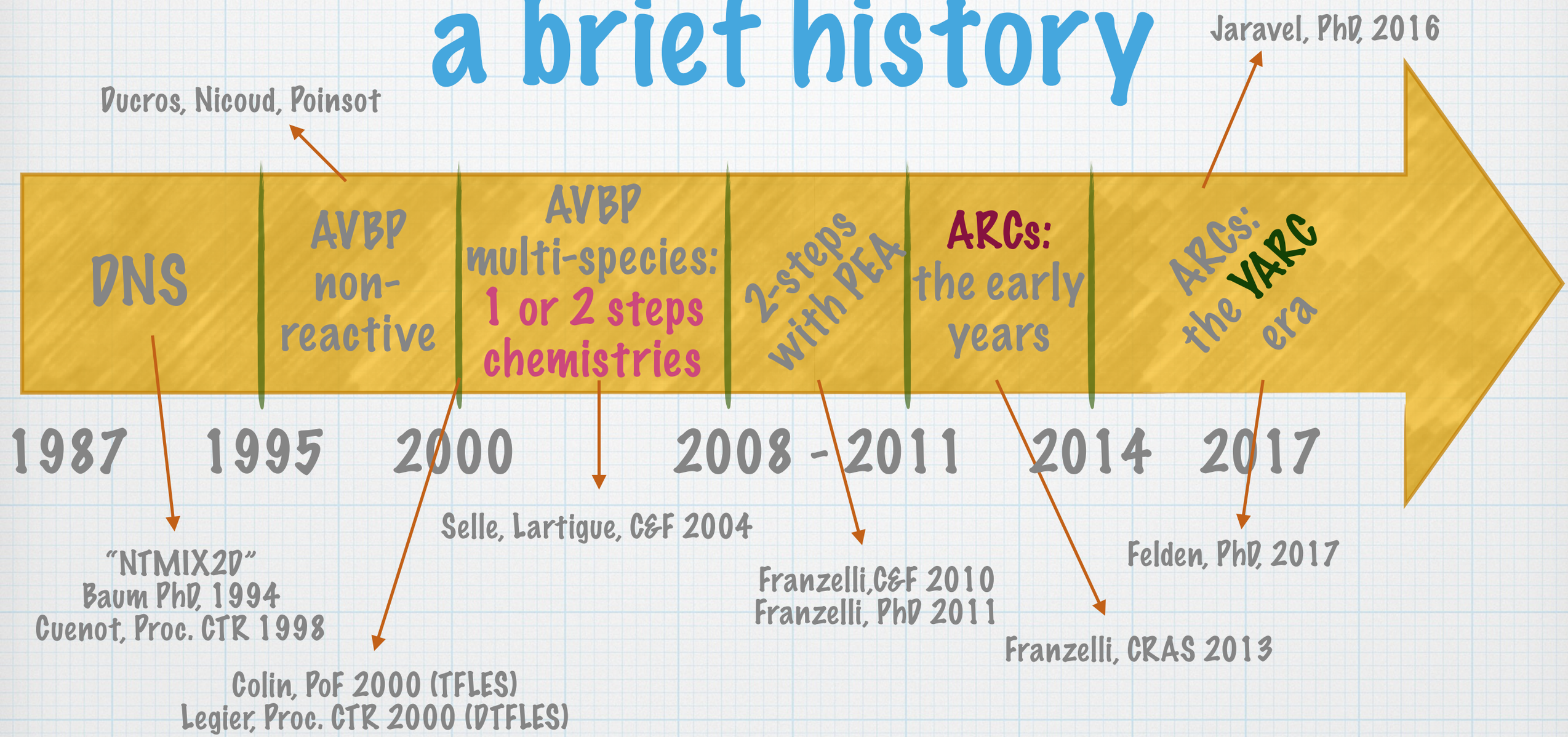
"ARC" in CFD (or how to take your simulations to the next level)

Anne Felden

11/09/2017



Chemistry in CERFACS: a brief history



—> So, "ARC" or Analytically Reduced Chemistry is a type of chemistry description ...

What exactly "ARC" ?

Reaction	A^a	n	E^a
$H + O_2 \rightleftharpoons OH + O$	3.52×10^{16}	-0.7	71.42
$H_2 + O \rightleftharpoons OH + H$	5.06×10^{4}	2.67	26.32
$H_2 + OH \rightleftharpoons H_2O + H$	1.17×10^{9}	1.3	15.21
$H_2O + O \rightleftharpoons 2OH$	7.06×10^{0}	3.84	53.47
$2H + M \rightleftharpoons H_2 + M^b$	1.30×10^{18}	-1.0	0.0
$H + OH + M \rightleftharpoons H_2O + M^b$	4.00×10^{22}	-2.0	0.0
$2O + M \rightleftharpoons O_2 + M^b$	6.17×10^{15}	-0.5	0.0
$H + O + M \rightleftharpoons OH + M^b$	4.71×10^{18}	-1.0	0.0
$O + OH + M \rightleftharpoons HO_2 + M^b$	8.30×10^{14}	0.0	0.0

Collection of elementary reactions: detailed mechanism

—> Directly derives from a "detailed" kinetic scheme

—> Only retains the "most important" chemistry information

—> Allows to capture finer chemistry details (NO, soot formation, fuel pyrolysis, auto-ignition, etc.) ,

—> Reasonable CPU cost

—> In essence:

1 or 2 steps chemistries =
- Cheap, reliable
- Basic features (sl, Tad)
- Low CPU cost


Renault Clio

ARCs =
- Cool useful options (Pollutant formation)
- Reasonable CPU cost


Nissan 370z

Detailed kinetics =
- Basically does everything ...
- Ridiculously overpriced CPU cost


Bugatti Chiron

+


Mercedes G (G63 AMG 6x6)

How do I derive these "ARCs" ?

* Several steps are required:

Detailed mechanism
(> 100 specs.)

(1)

—> Start with a detailed mechanism adapted to your needs
—> Determine targeted type of applications (premixed/diffusion, secondary dilution etc.)
—> **Determine operating range** (lean/rich, T range, etc.)
—> **Define targets** (soot precursors, NO, etc.)

(2)

—> **Remove "unnecessary" species**
—> **Remove "unnecessary" reactions**
—> Regroup information (lumping)

Skeletal mechanism
(10-40 specs.)

(3)

—> **Spot species with short lifespan**
—> Spot species in small concentrations
—> Re-express the concentrations of these short living species

ARC
(10-30 specs.)

(Loose the " " because now, the meaning of ARC is cristal clear)

How do I use these ARCs in my CFD solver ?

* (Again) several steps are required:

—> Ensure the validity of your ARC : use a chemistry solver !!

—> Format the ARC properly:

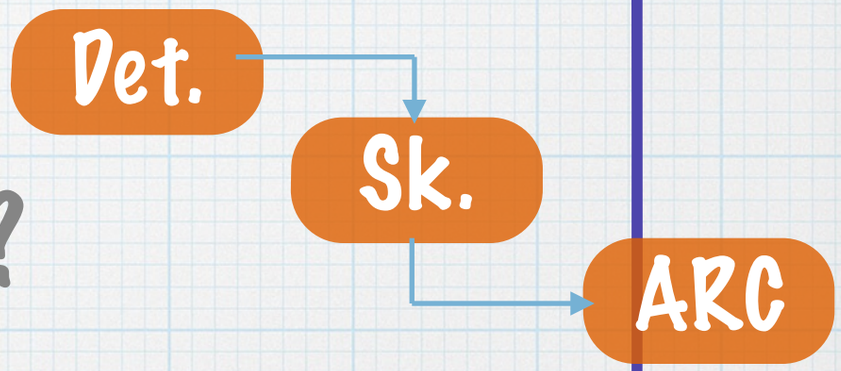
- Requires an external routine for the computation of the transported species
- Often requires transport properties simplifications
- Might require specific stiffness management

Let's be specific

So far we have seen:

Nissan 370z

* What exactly is an "ARC" ?
* How do I derive these "ARCs" ?
* How do I use these ARCs in my CFD solver ?



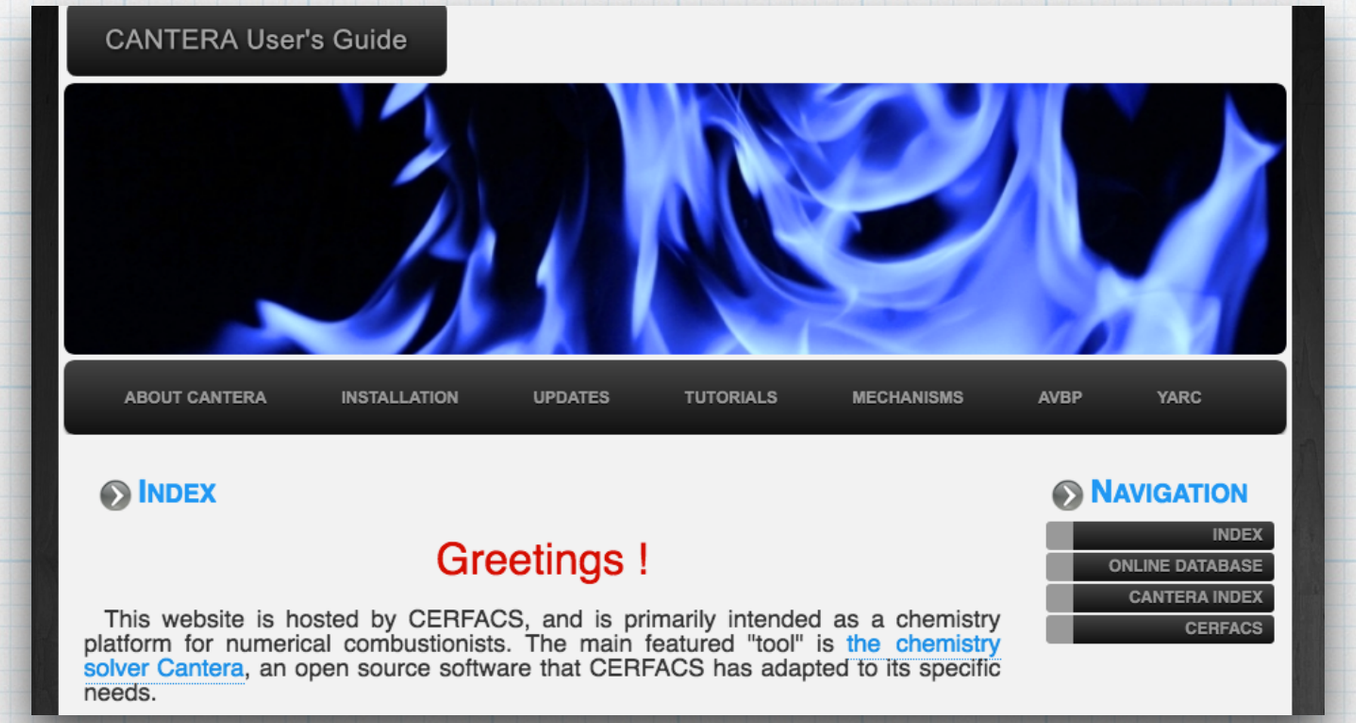
Yes !!

→ Can I do/learn more about all of this at CERFACS ?

ARC resources in the CFD CERFACS team

* What exactly is an "ARC" ?

—> Learn all about it online: www.cerfacs.fr/cantera



—> Read dedicated PhD thesis:

https://pepiot.mae.cornell.edu/pdf/Pepiot_Thesis.pdf (P. Pepiot)

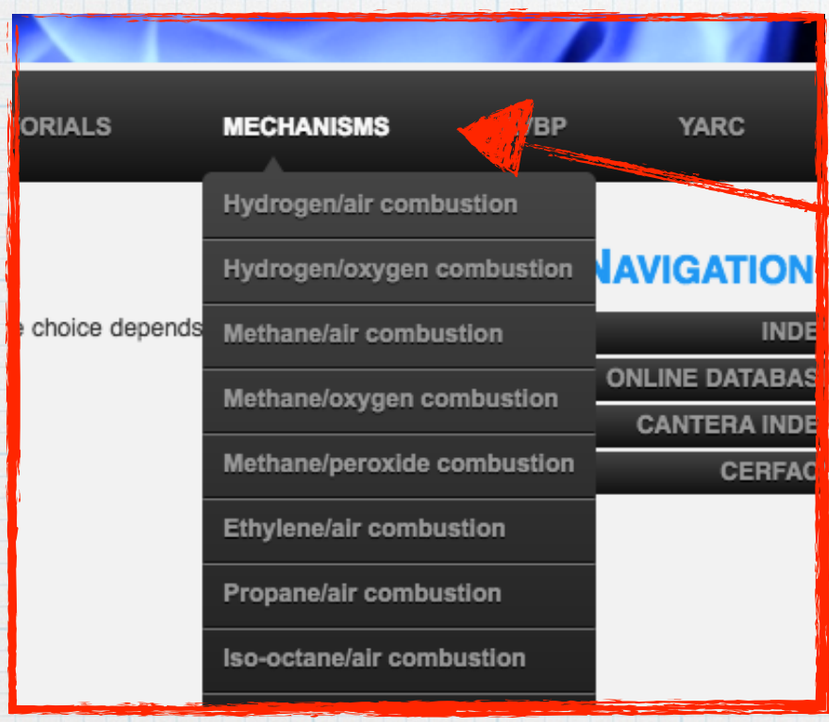
http://cerfacs.fr/wp-content/uploads/2017/08/CFD_THESE_FELDEN.pdf (A. Felden)

http://cerfacs.fr/wp-content/uploads/2016/06/THESE_CFD_JARAVEL.pdf (T. Jaravel)

ARC resources in the CFD CERFACS team

* How do I derive these "ARCs" ?

—> You don't necessarily have to... Check out the "mechanisms" section of the cerfacs website: http://www.cerfacs.fr/cantera/mechanisms/ maybe there already your needs



—> If you need a "new" ARC: **use YARC !!** Learn all about it on the YARC tutorial online: www.cerfacs.fr/cantera/YARC/First_Tutorial.php. Also, use a detailed mechanism featured/referenced on the website !!

ARC resources in the CFD CERFACS team

* How do I use these ARCs in my CFD solver?

—> Ensure the validity of ARC with CANTERA !! Check the "installation" section www.cerfacs.fr/cantera/installation.php and the tutorials from the CERFACS' CANTERA formation www.cerfacs.fr/cantera/docs/tutorials/CANTERA_HandsOn.pdf

ABOUT CANTERA | INSTALLATION | UPDATES | TUTORIALS | MECHANISMS | AVBP | YARC

INSTALLATION

There are two different versions of Cantera at Cerfacs , both **pre-compiled and ready to use** :

- The 1.8 version, modified to inculde a simplified transport model (constant Sc and Pr numbers) and be able to deal with analytically reduced chemistry (ARC).
- And the more recent 2.1.1 version, also modified.

There is also currently **development on a more recent version (2.3), available via the CERFACS GitLab**. E-mail felden@cerfacs.fr or lapeyre@cerfacs.fr if you want to get involved ! :

Note that you should use the version 2.1.1 as much as possible, as this is the stable version !! Additionally, frequently visit the 'Updates' section, to keep informed about the latest developments in the CERFACS version of the code !

NAVIGATION
- INDEX
- ONLINE DATABASE
- CANTERA INDEX
- CERFACS

CANTERA User's Guide

ABOUT CANTERA | INSTALLATION | UPDATES | TUTORIALS | MECHANISMS | AVBP | YARC

INDEX

Greetings !

This website is hosted by CERFACS, and is primarily intended as a chemistry platform for numerical combustionists. The main featured "tool" is the chemistry solver Cantera, an open source software that CERFACS has adapted to its specific needs.

NAVIGATION
- INDEX
- ONLINE DATABASE
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- CERFACS

USEFUL DOCUMENTATION

CERFACS Resources:

- A quick presentation of Cantera.
- Tutorials from the CERFACS' Cantera formation.
- Help for the tutorials from the CERFACS' Cantera formation.

Web Resources:

- Official Cantera Documentation: This site contains documentation for the cur
- The Cantera SourceForge site: Distribution of Cantera releases and binary in history.
- Official Cantera discussion group: This site has a message board for discuss **is a lifesaver !**

Note: The CANTERA formation is in NOVEMBER !

ARC resources in the CFD CERFACS team

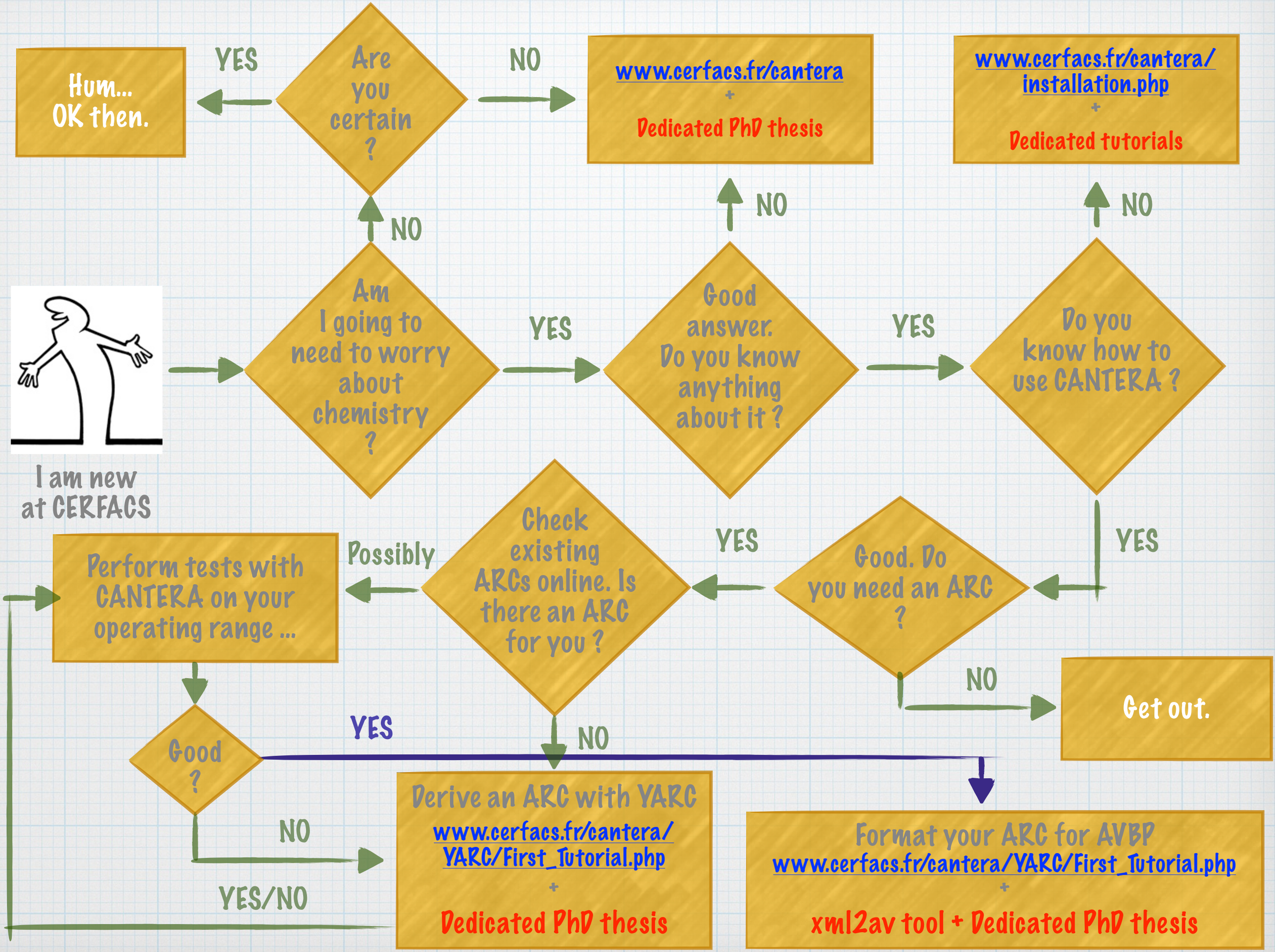
* How do I use these ARCs in my CFD solver?

—> Format the ARC properly !! Use a "f90" routine. Find it online if you use an already existing mechanism. Learn all about it on the YARC tutorial online: www.cerfacs.fr/cantera/YARC/First_Tutorial.php.

—> Simplified "AVBP" transport: find proper constant values of Pr and Sc numbers. Use the xml2av tool or find it online if you use an already existing mechanism.

—> Stiffness control ?

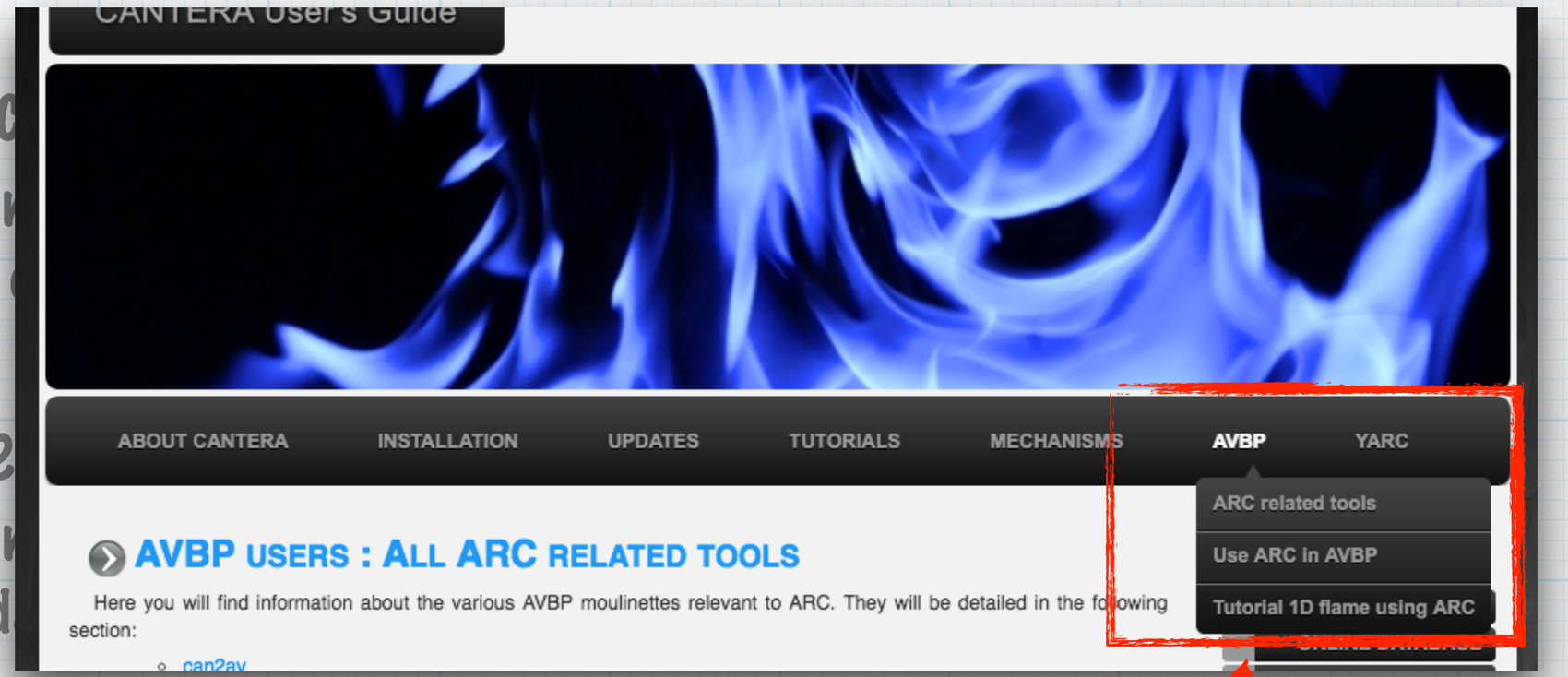
- Use a "sub-cycling" or control the time step directly in AVBP. Check-out the AVBP website: http://www.cerfacs.fr/avbp7x/HELP/avbphelp.php
- "Implicit" the computation of some stiff but necessary transported species. Check-out the PhD thesis of A. Felden: http://cerfacs.fr/wp-content/uploads/2017/08/CFD_THESE_FELDEN.pdf


I am new at CERFACS
Are you certain ?
YES
Hum... OK then.
NO
www.cerfacs.fr/cantera + Dedicated PhD thesis
Am I going to need to worry about chemistry ?
NO
YES
Good answer. Do you know anything about it ?
NO
YES
Do you know how to use CANTERA ?
NO
www.cerfacs.fr/cantera/installation.php + Dedicated tutorials
YES
Good. Do you need an ARC ?
NO
Get out.
YES
Check existing ARCs online. Is there an ARC for you ?
Possibly
Perform tests with CANTERA on your operating range ...
Good ?
YES
NO
Derive an ARC with YARC
www.cerfacs.fr/cantera/YARC/First_Tutorial.php + Dedicated PhD thesis
Format your ARC for AVBP
www.cerfacs.fr/cantera/YARC/First_Tutorial.php + xml2av tool + Dedicated PhD thesis
NO
YES/NO

What is next ?

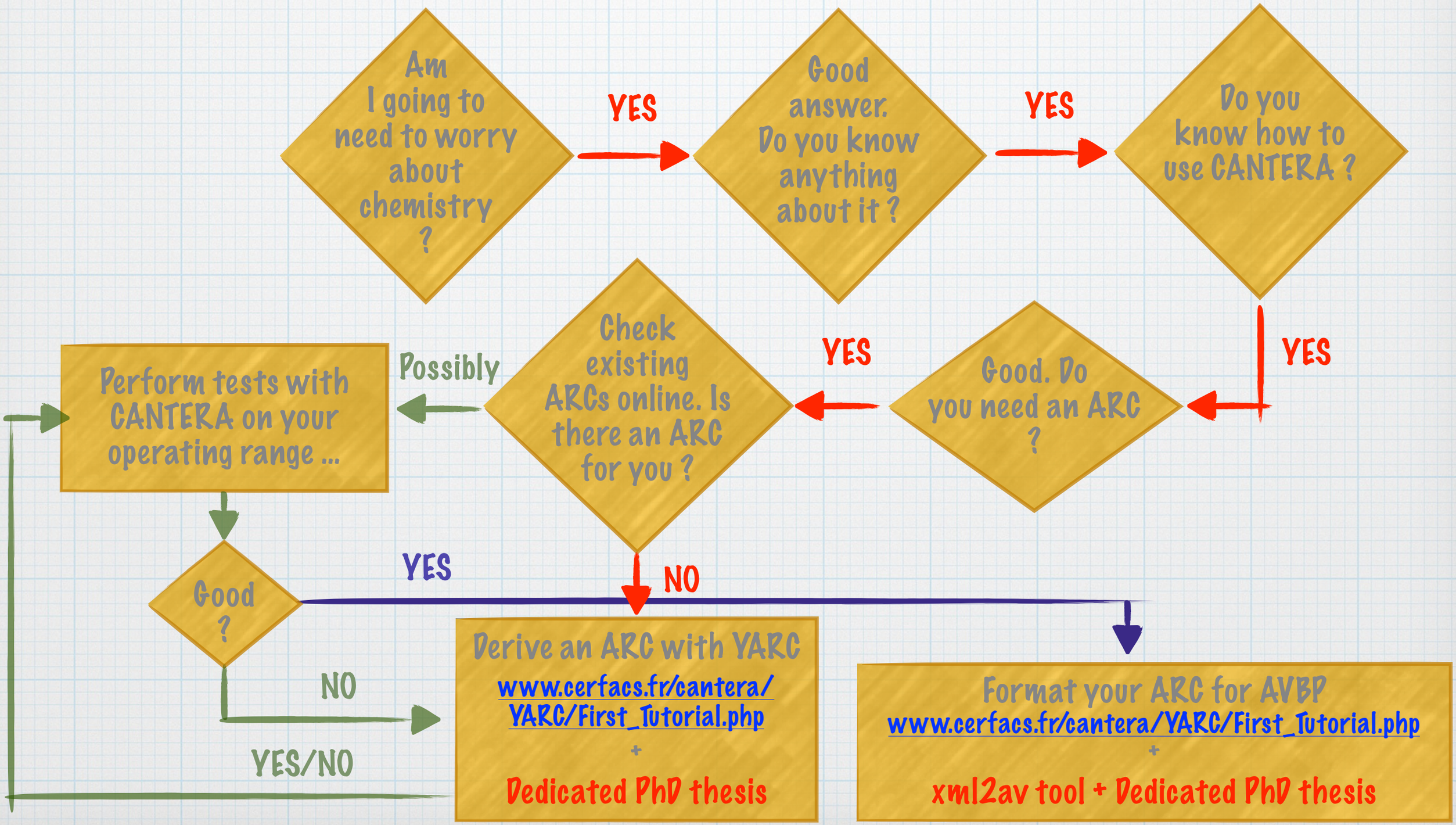
—> In AVBP:

* Initialize your c
  —> can2av (1D ar
  —> glob2arc (3D
* Control stiffne
  —> Use sub-cyclin
  in mixture_d
* Monitor your computation:
  —> In time: tool xm & tool x_mc_spec_exact
* Visualize chemistry-related stuff:
  —> Store selected source terms in instantaneous and average solutions with run.params keyword "save_source_spec"



Find dedicated AVBP "ARC tools" section online

An example !


Am I going to need to worry about chemistry ?
YES
Good answer. Do you know anything about it ?
YES
Do you know how to use CANTERA ?
YES
Good. Do you need an ARC ?
YES
Check existing ARCs online. Is there an ARC for you ?
Possibly
Perform tests with CANTERA on your operating range ...
Good ?
YES
NO
NO
YES/NO
Derive an ARC with YARC
www.cerfacs.fr/cantera/YARC/First_Tutorial.php
+
Dedicated PhD thesis
Format your ARC for AVBP
www.cerfacs.fr/cantera/YARC/First_Tutorial.php
+
xml2av tool + Dedicated PhD thesis

An example !

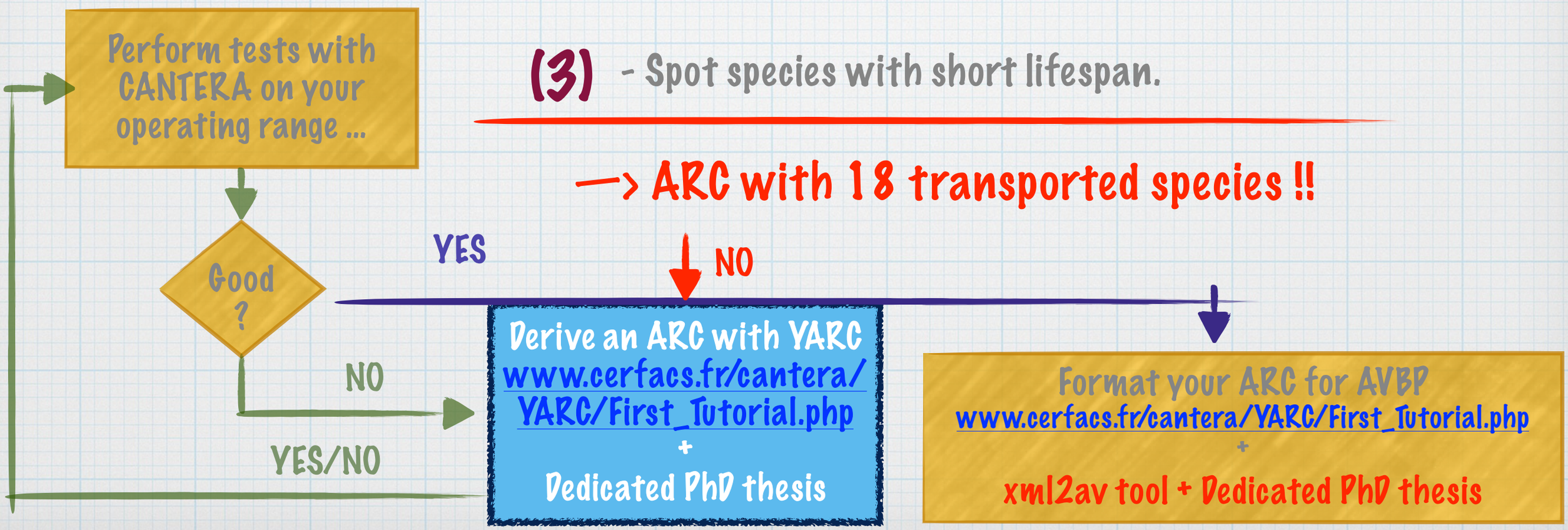
(1) - Choose an adapted detailed mechanism: Narayanaswamy, C&F 2010 for ethylene/ air combustion. Contains 158 species.

- Choose targets and operating range: partially-premixed combustion, soot investigations

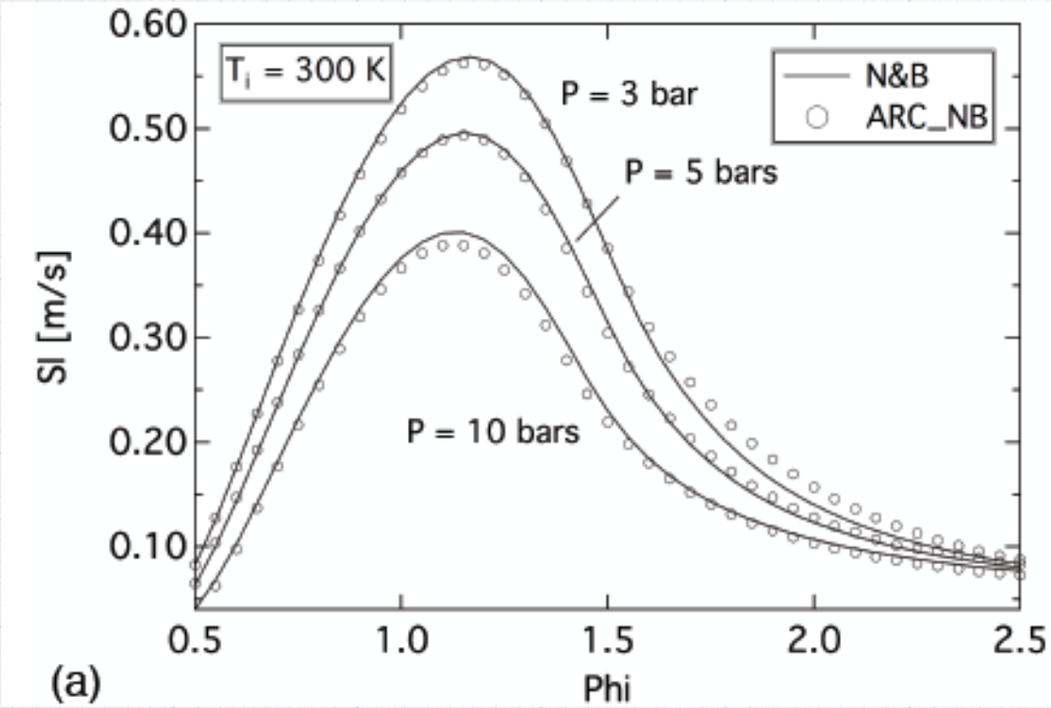
(2) - Remove unnecessary reactions and species.

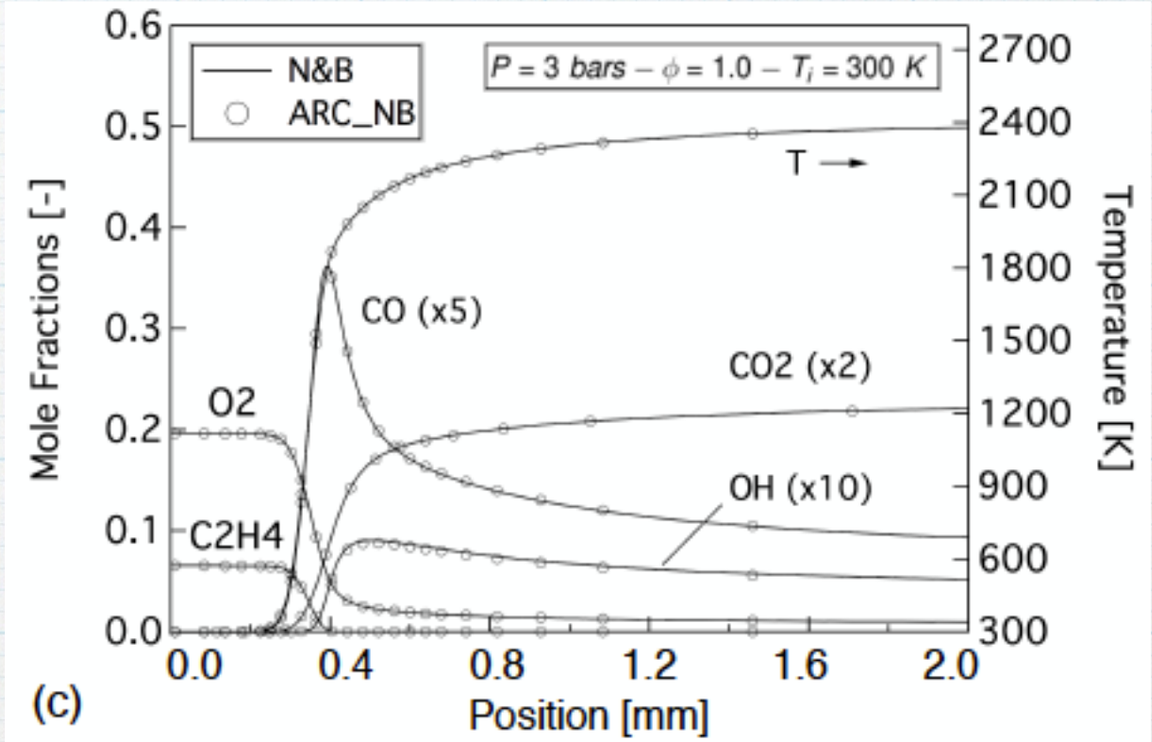
(3) - Spot species with short lifespan.

—> ARC with 18 transported species !!



An example !





Perform tests with CANTERA on your operating range ...

Good ?

YES

NO

YES/NO

Derive an ARC with YARC

www.cerfacs.fr/cantera/YARC/First_Tutorial.php

+

Dedicated PhD thesis

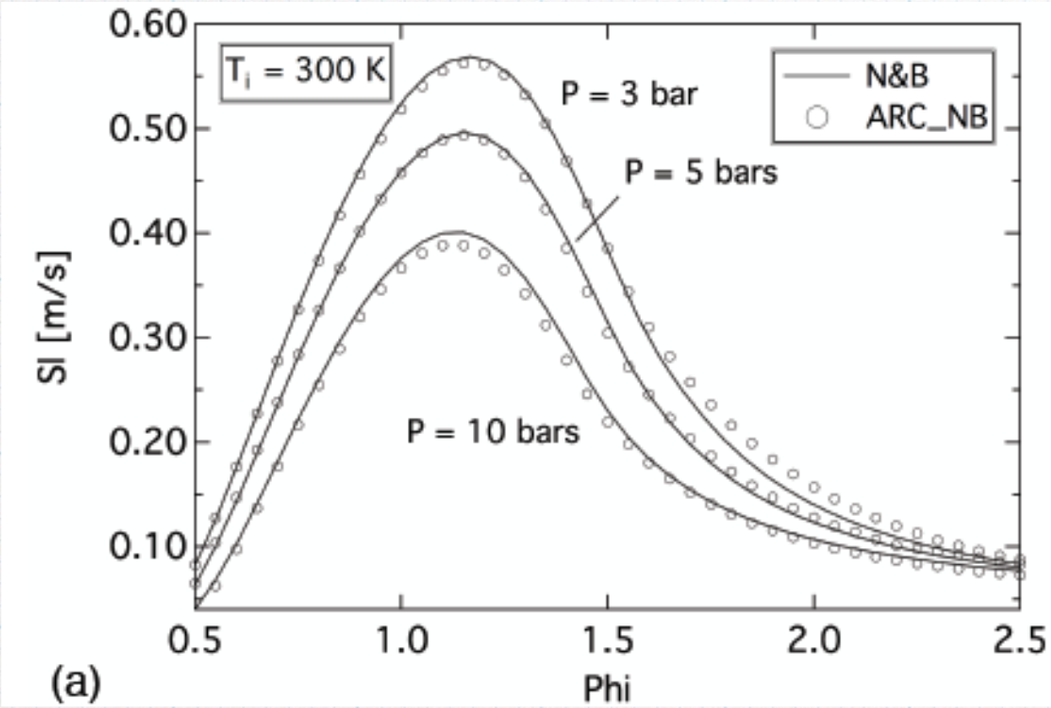
Format your ARC for AVBP

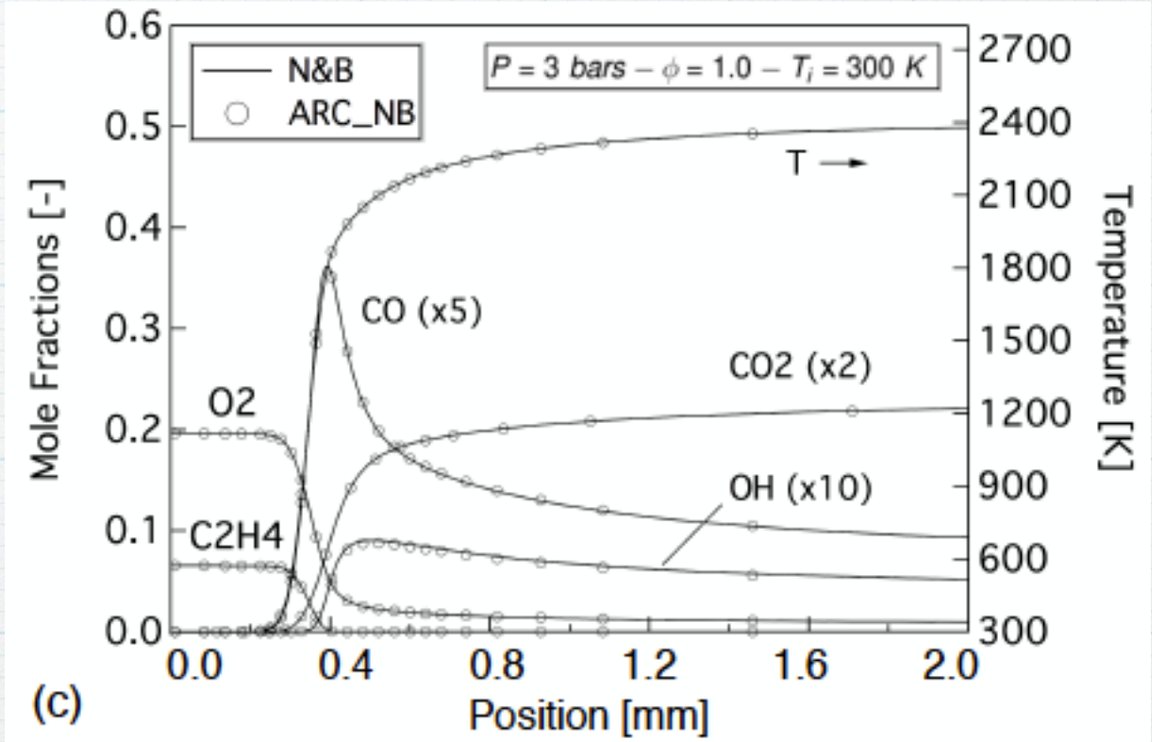
www.cerfacs.fr/cantera/YARC/First_Tutorial.php

+

xml2av tool + Dedicated PhD thesis

An example !





Perform tests with CANTERA on your operating range ...

Good ?

YES

NO

YES/NO

Derive an ARC with YARC

www.cerfacs.fr/cantera/YARC/First_Tutorial.php

+

Dedicated PhD thesis

Format your ARC for AVBP

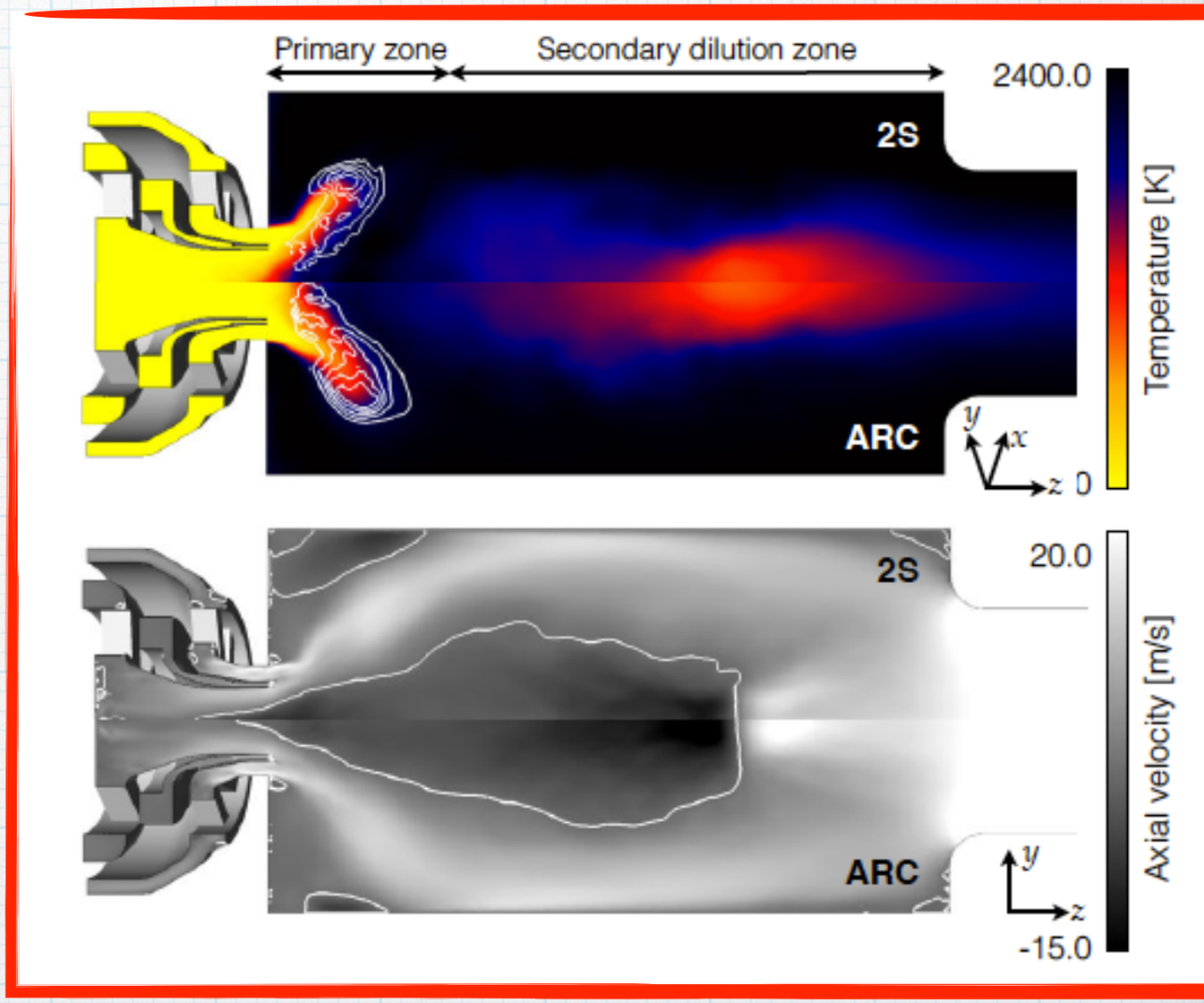
www.cerfacs.fr/cantera/YARC/First_Tutorial.php

+

xml2av tool + Dedicated PhD thesis

An example !

- Obtain "mixture_database" and "species_database" with xml2av
- Obtain "f90" routine with YARC
- Initialize computation from 2S simulation with glob2arc !
- Visualize !



Perform tests with CANTERA on your operating range ...

Good ?

YES

NO

YES/NO

Derive an ARC with YARC
www.cerfacs.fr/cantera/YARC/First_Tutorial.php
+
Dedicated PhD thesis

Format your ARC for AVBP
www.cerfacs.fr/cantera/YARC/First_Tutorial.php
+
xml2av tool + Dedicated PhD thesis

Compilation of resources:

—> Online:

www.cerfacs.fr/cantera CERFACS CANTERA website
www.cerfacs.fr/cantera/docs/tutorials/CANTERA_HandsOn.pdf Exhaustive CANTERA Hands-On
www.cerfacs.fr/cantera/installation.php Use CANTERA at CERFACS
www.cerfacs.fr/cantera/YARC/First_Tutorial.php YARC tutorial
NOTE: YARC/AVBP sections online are protected by password !!!
(—> ask felden@cerfacs.fr)

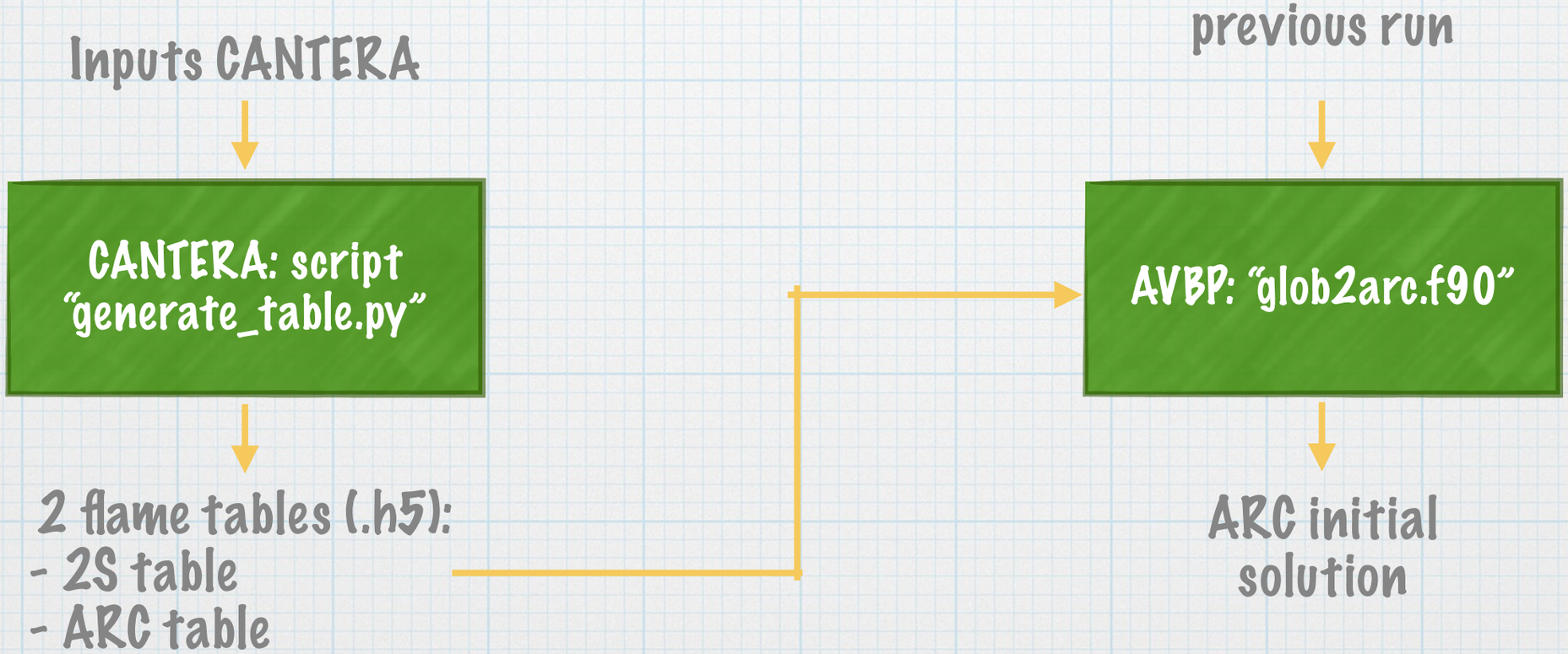
—> PhD thesis:

https://pepiot.mae.cornell.edu/pdf/Pepiot_Thesis.pdf (P. Pepiot)
http://cerfacs.fr/wp-content/uploads/2017/08/CFD_THESE_FELDEN.pdf (A. Felden)
http://cerfacs.fr/wp-content/uploads/2016/06/THESE_CFD_JARAVEL.pdf (T. Jaravel)

Moulinette: glob2arc

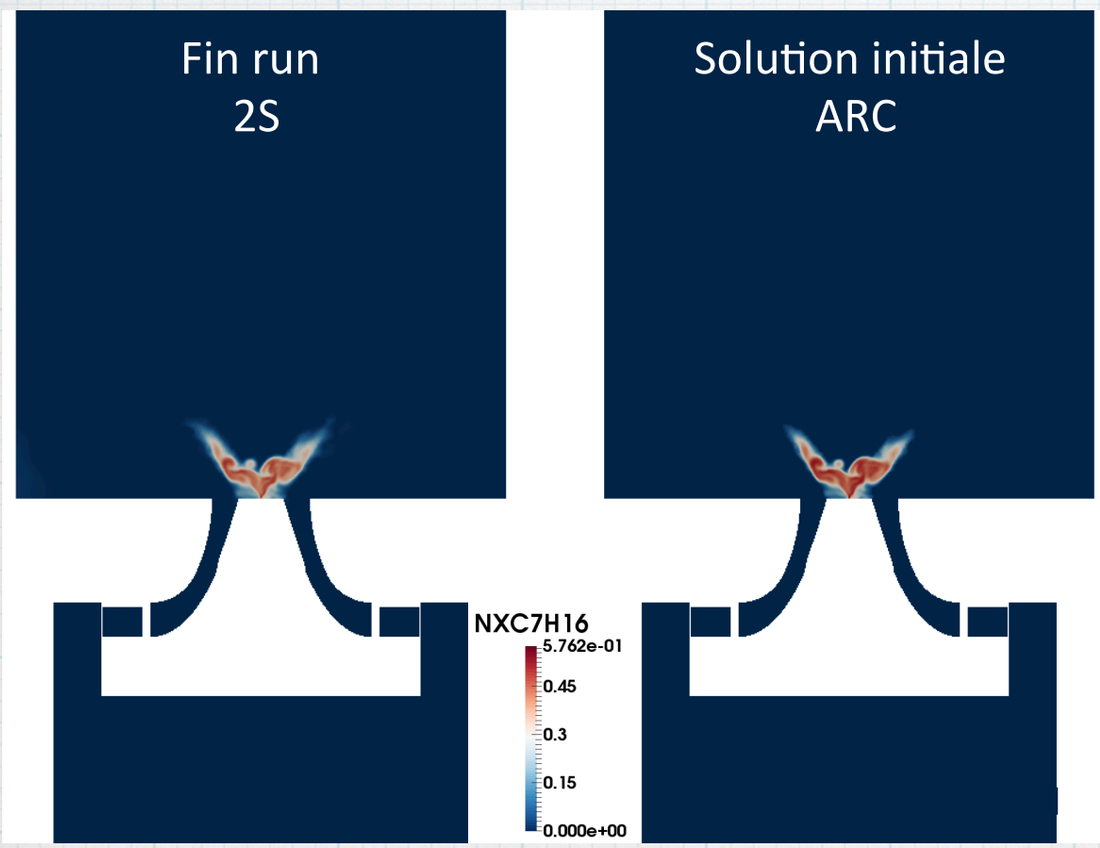
—> Why this tool ?

- Initialize ARC computation from global mechanism computation
- Shorten the transient period
- IT REQUIRES CANTERA with ARC features !



Moulinette: glob2arc

—> Example of use:



From F. Colin

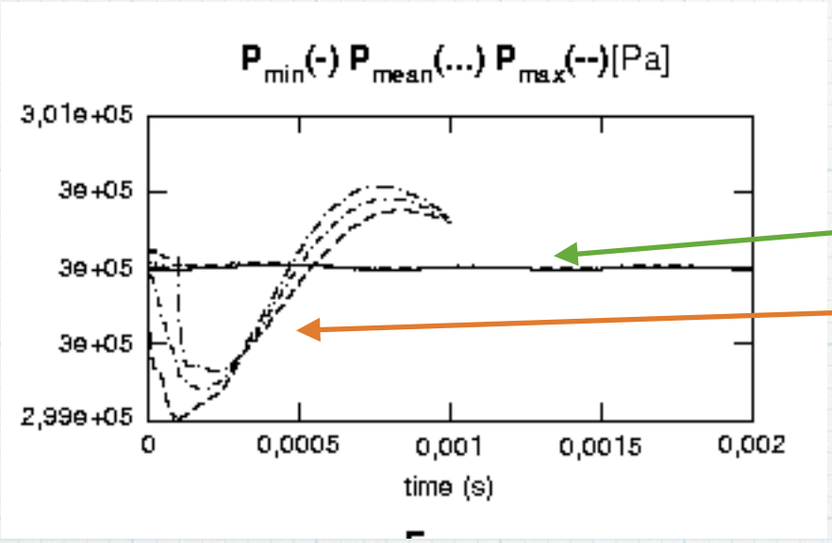
—> No sub-cycling necessary (with add_spec: necessary)

—> Requires some user input !!

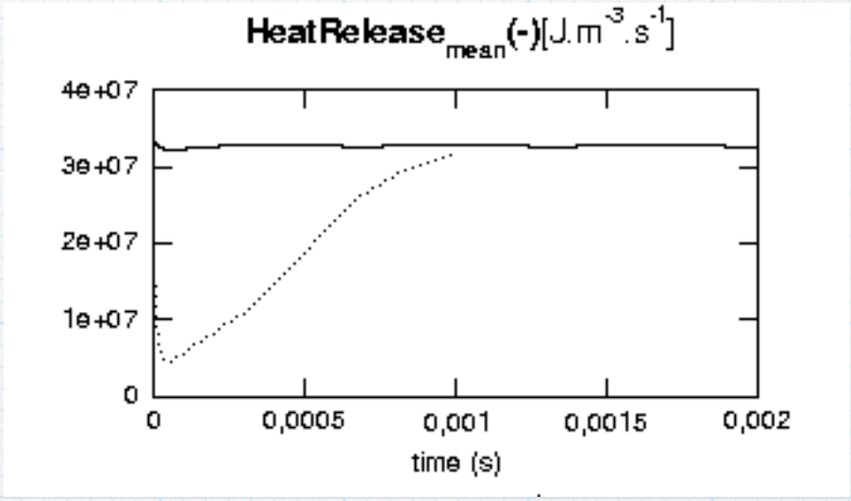
- Discretization of the .h5 chemistry tables
- Management of the "pure" fuel stream

Moulinette: glob2arc

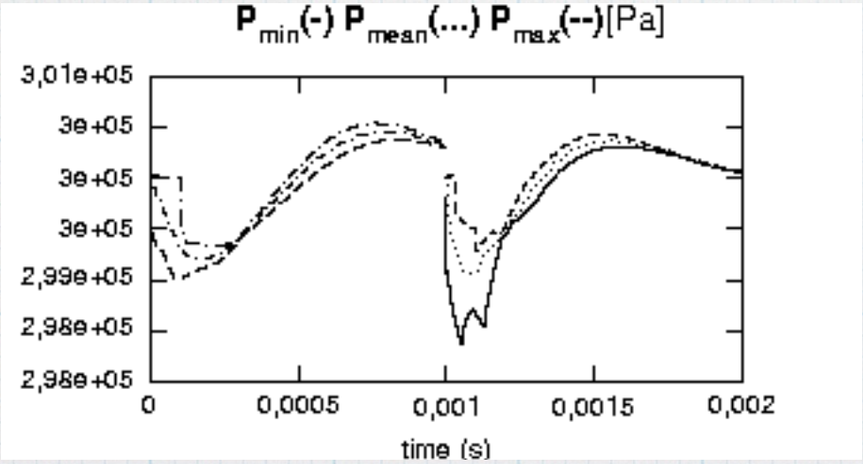
—> Example of use: 1D flame C2H4 Phi 0.8 P,T atm



can2av VS
glob2arc



ARC



addspec VS
glob2arc