# Stoichiometric projection methods for plasma simulations

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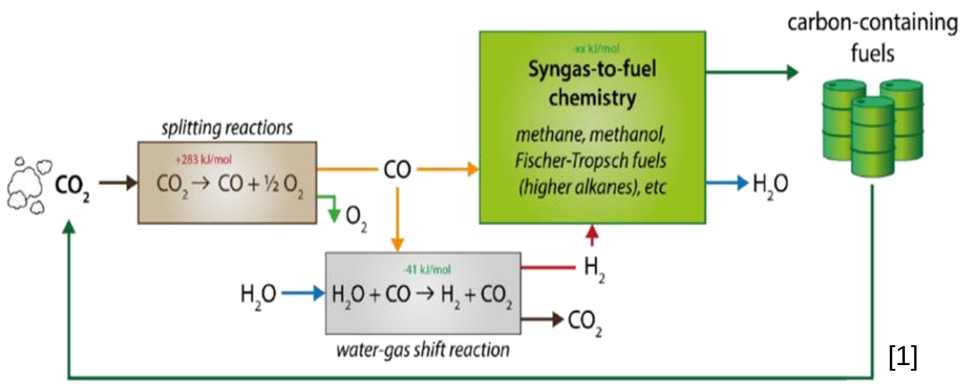
## Introduction

**Goal: $CO_2$ decomposition with plasmas for synthetic fuel processing**

**Numerical simulation challenge: >70 components, >5000 reactions[2]**

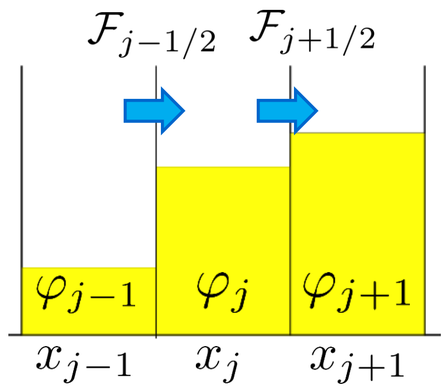



[1]

## 2. System of conservation laws

***Drift-Diffusion-Reaction system (continuous)***

$$\frac{d}{dx}\underbrace{\left(\boldsymbol{u}\varphi - \boldsymbol{\mathcal{E}}\frac{d\varphi}{dx}\right)}_{:=\mathcal{F}(\varphi)} = \boldsymbol{s}(\varphi)$$




***Drift-Diffusion-Reaction system (discrete)***

$$\mathcal{F}_{j+1/2} - \mathcal{F}_{j-1/2} = \Delta x \boldsymbol{s}(\boldsymbol{\varphi}_j)$$

## 3. Argon plasma test case

***Stoichiometric projection: decouple system in conserved variables and others[3]***

***1 Reaction, 3 species***

$$\mathrm{Ar} \rightleftharpoons \mathrm{Ar}^+ + \mathrm{e}^-,$$

***Stoichiometry: 2 constraints on sources***

1.Charge conservation

$$s_{Ar^+} - s_{e^-} = 0$$

2. Argon conservation

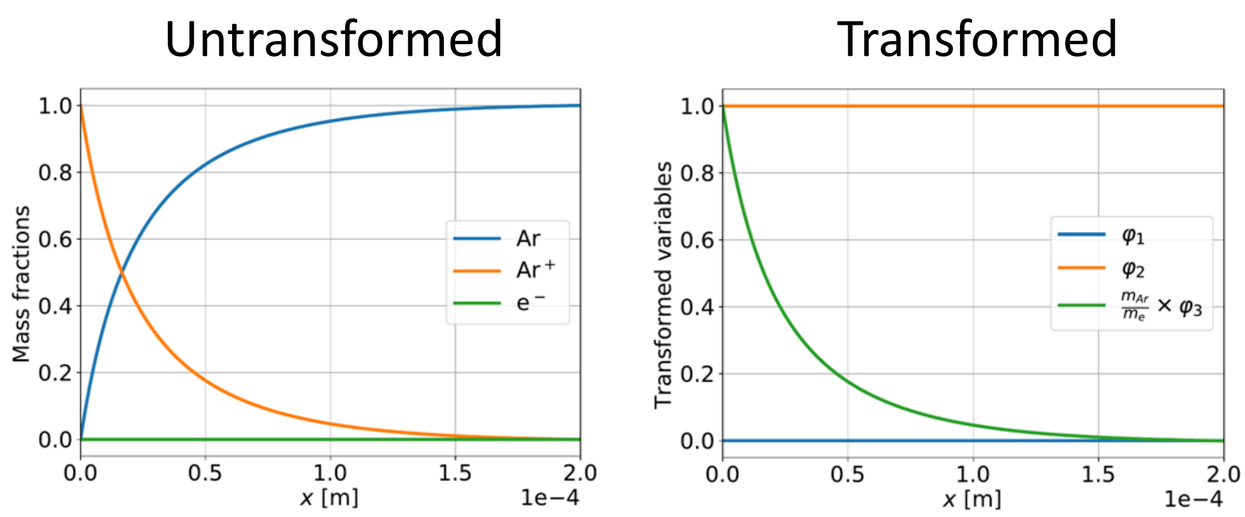
$$s_{Ar} + s_{Ar^+} = 0$$

***Linear transformation of original equation set***

$$\begin{aligned} \frac{d\mathcal{F}_{Ar}}{dx} &= s_{Ar} \\ \frac{d\mathcal{F}_{Ar^+}}{dx} &= s_{Ar^+} \\ \frac{d\mathcal{F}_{e^-}}{dx} &= s_{e^-} \end{aligned} \quad \Rightarrow \quad \begin{aligned} \frac{d}{dx}\left(\mathcal{F}_{Ar^+} - \mathcal{F}_{e^-}\right) &= 0 \qquad \varphi_1 \\ \frac{d}{dx}\left(\mathcal{F}_{Ar} + \mathcal{F}_{Ar^+}\right) &= 0 \qquad \varphi_2 \\ \frac{d\mathcal{F}_{e^-}}{dx} &= s_{e^-} \qquad \varphi_3 \end{aligned}$$

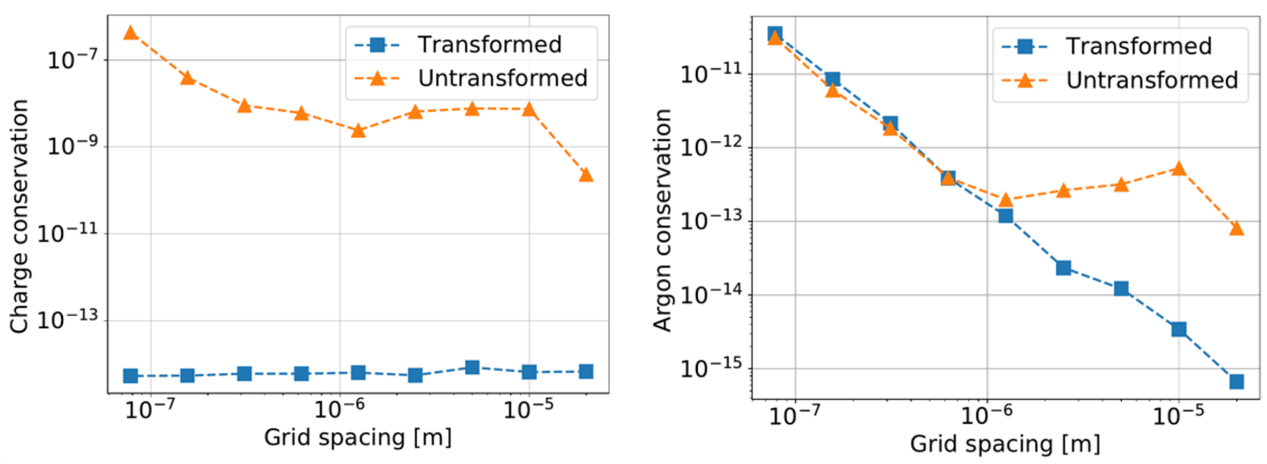
Untransformed Transformed

Untransformed Transformed

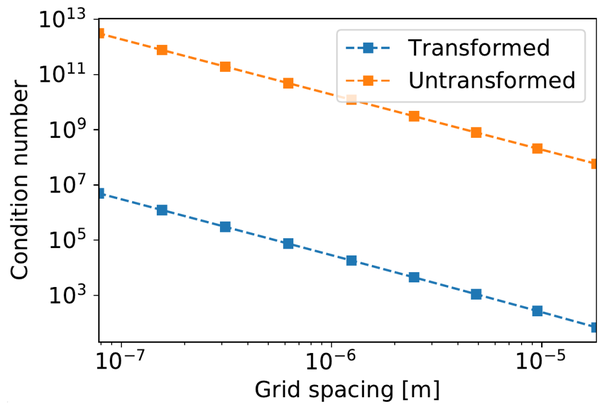



## 4. Numerical results argon case

***Charge & argon conservation improved***




***Condition number discretization matrix decreased***




*Smaller condition number:*
*- Less sensitive to arithmetic errors*
*- Faster convergence of iterative linear solvers*

## 5. Conclusion & outlook

***- Stoichiometry used to transform system***

***- Transformed system partly source-free***

***- Numerically favorable properties for example system***

***- Apply to complex chemistry ($CO_2$)***

***- Exploit source-free set in solution procedure***

***- Transformation not unique, further optimization possible?***

## Acknowledgements

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[1] Vibrational excitation for efficient chemistry in CO2 microwave plasmas van den Bekerom, D.C.M.

[2] Koelman, P. (2019). Chemical aspects of CO2 plasma modelling

[3] Krautle, Knabner (2007) A reduction scheme for the coupled multicomponent transport-reaction problems in porous media