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Stoichiometric projection methods for plasma simulations

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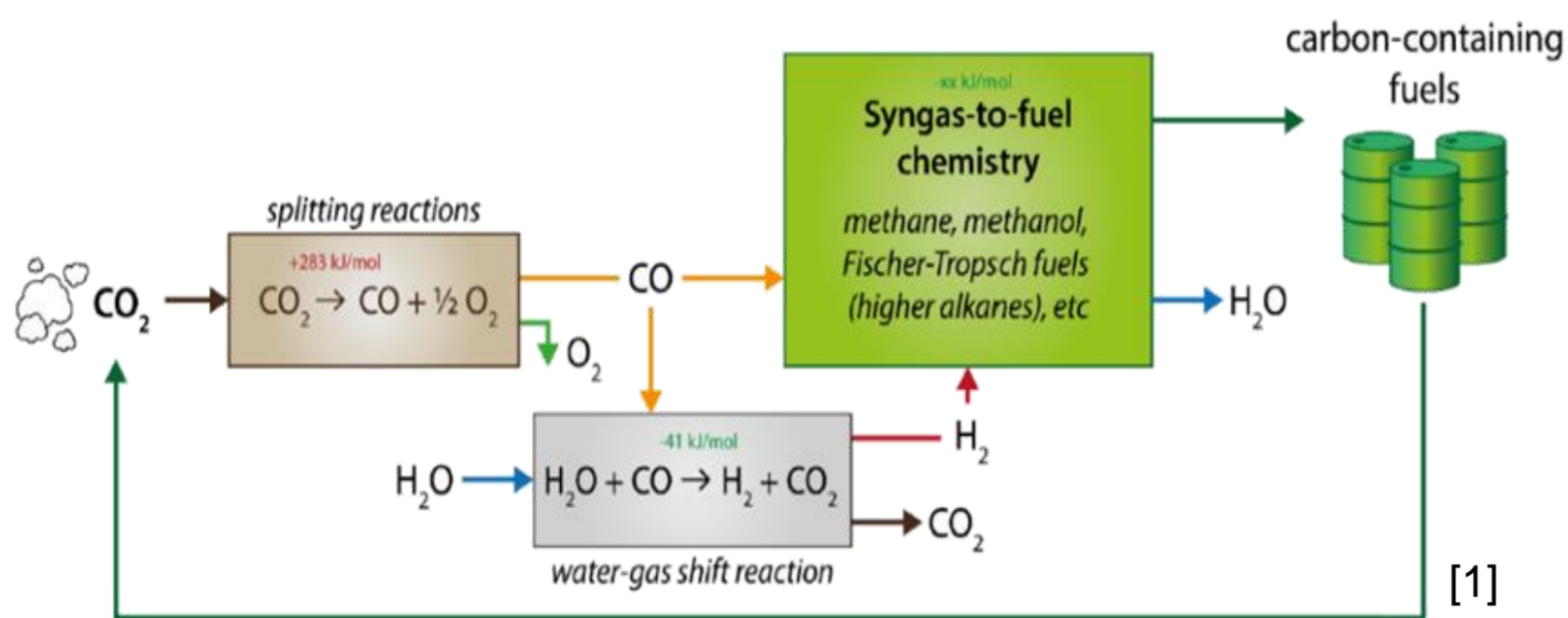
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Introduction

Goal: CO₂ decomposition with plasmas for synthetic fuel processing
Numerical simulation challenge: >70 components, >5000 reactions^[2]

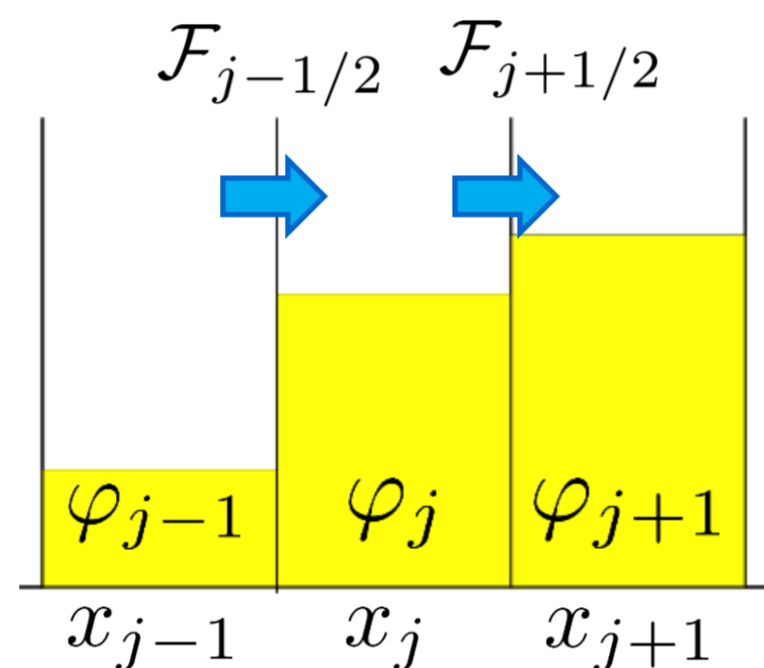


2. System of conservation laws

Drift-Diffusion-Reaction system (continuous)

$$\frac{d}{dx} \left(u\varphi - \mathcal{E} \frac{d\varphi}{dx} \right) = s(\varphi)$$

$$:= \mathcal{F}(\varphi)$$



Drift-Diffusion-Reaction system (discrete)

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

3. Argon plasma test case

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

1 Reaction, 3 species



Stoichiometry: 2 constraints on sources

1. Charge conservation

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

2. Argon conservation

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

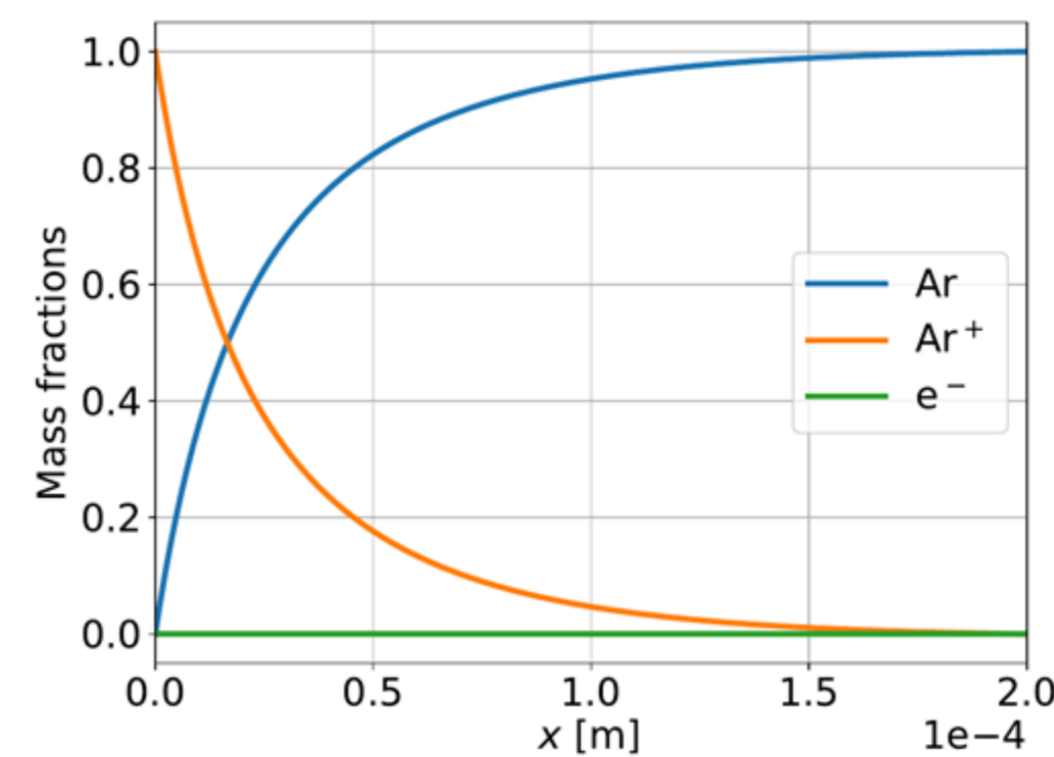
Linear transformation of original equation set

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

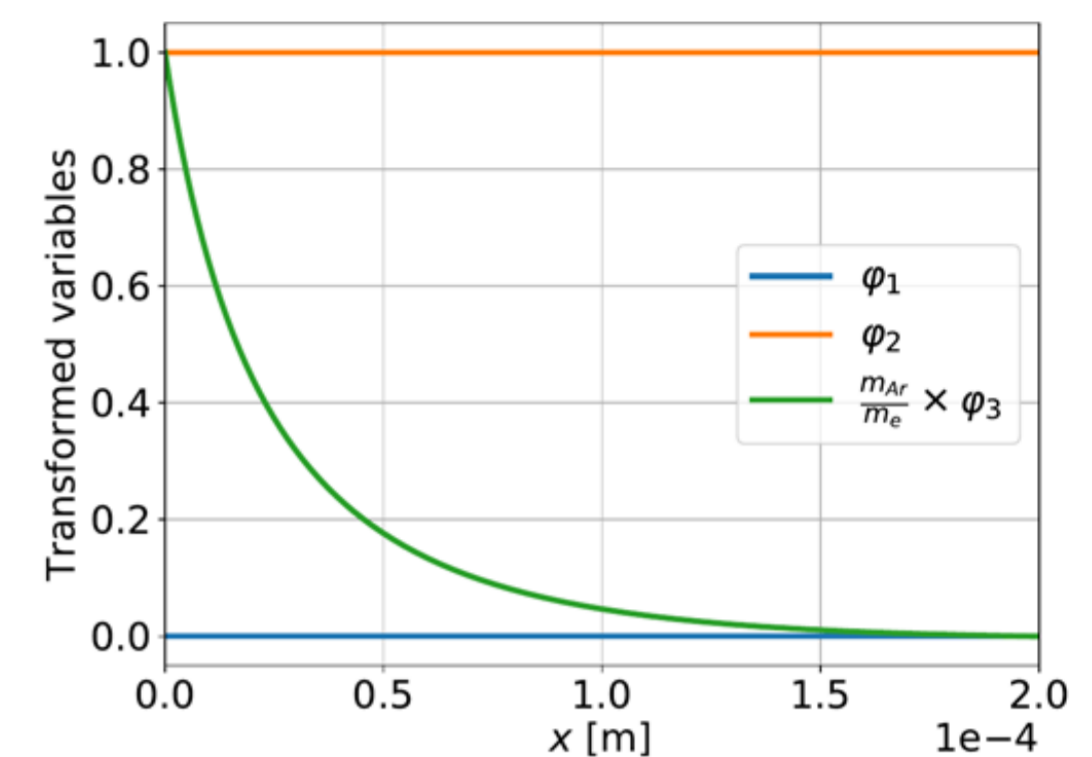
Untransformed

Transformed

Untransformed

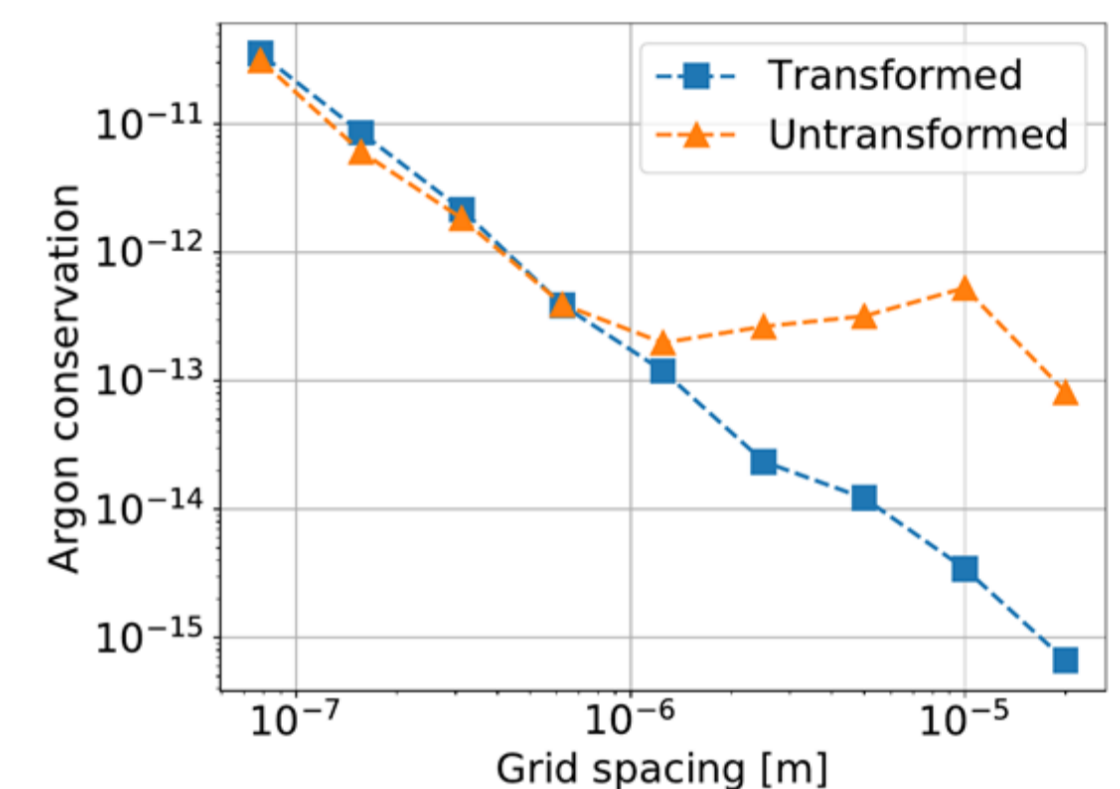
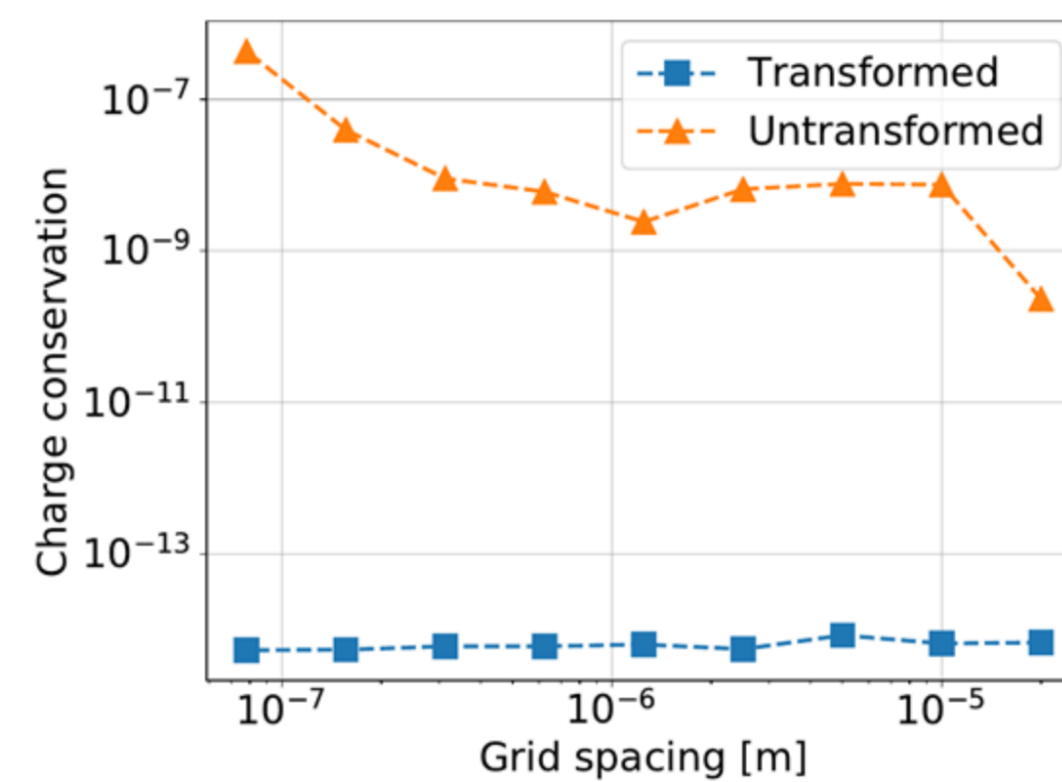


Transformed

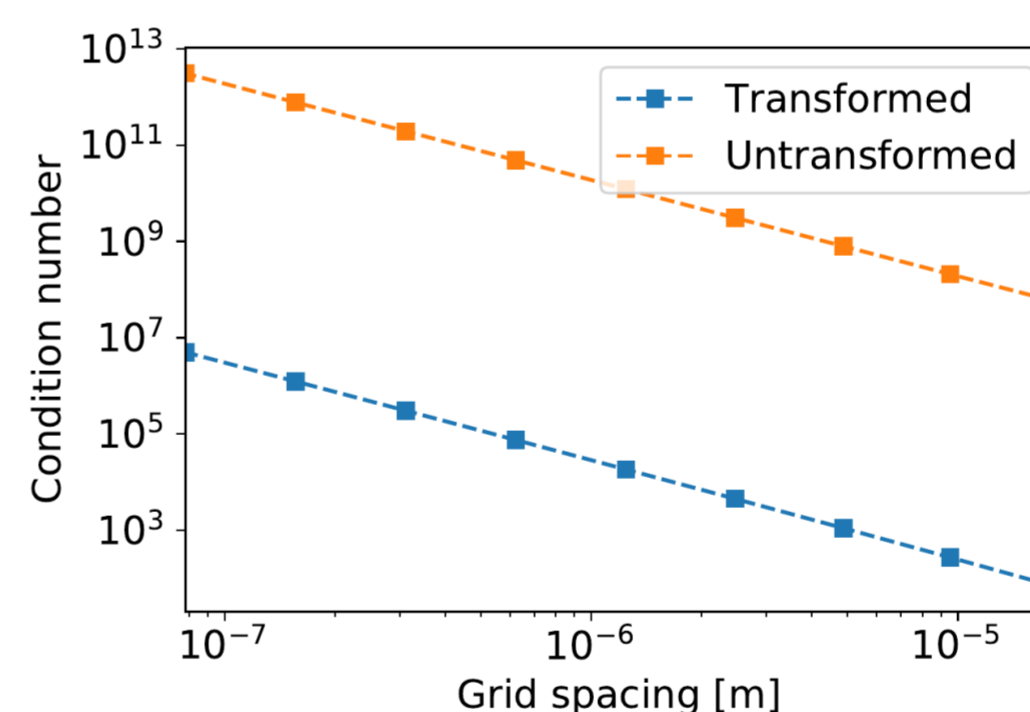


4. Numerical results argon case

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 (CO₂)
- 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