Zero-dimensional Stochastic Modeling of Chemical Kinetics

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LOGE
LUND COMBUSTION ENGINEERING

Outline

- About the company

- Chemical kinetics

- The 0D Stochastic Reactor Model

- Mathematical applications

- Growing up

- The employer's perspective

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About the company

- Founded in 2005 by prof. Fabian Mauss as a spin-off from a university project.

- Approx. 10 employees in Lund, Sweden and Cottbus, Germany.

- Specialists in simulating chemical kinetics.

- Software development as well as consultancy projects.

Chemical kinetics

- The overlap between chemistry and physics – reacting flows!
- Typically extremely time-consuming to solve numerically.
- Our 0D Monte Carlo model offers a time-efficient tool to solve many problems, for example related to combustion engines.

Bjerkborn – Zero-dimensional Stochastic Modeling of Chemical Kinetics
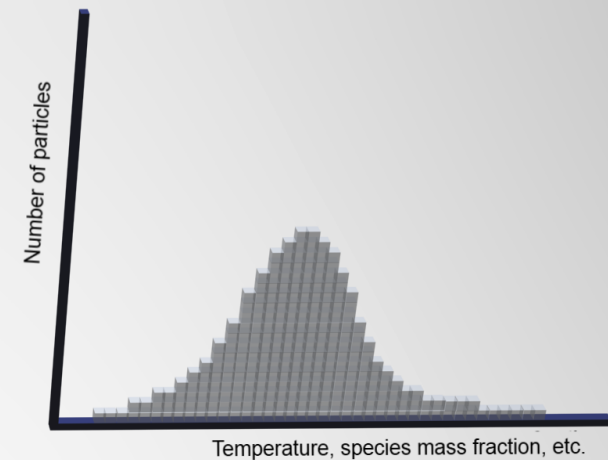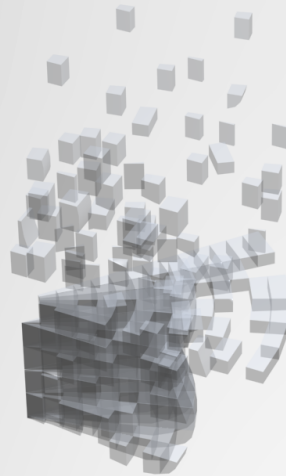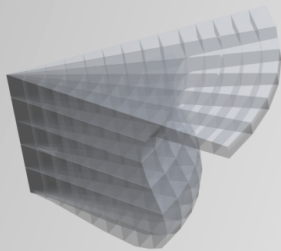
Chemical kinetics

- By studying the gas as discrete particles without spatial resolution, we aim to study the development of realizations of the PDF.

- Disregarding the spatial flow allows us to use much more precise chemistry models!

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The 0D Stochastic Reactor Model
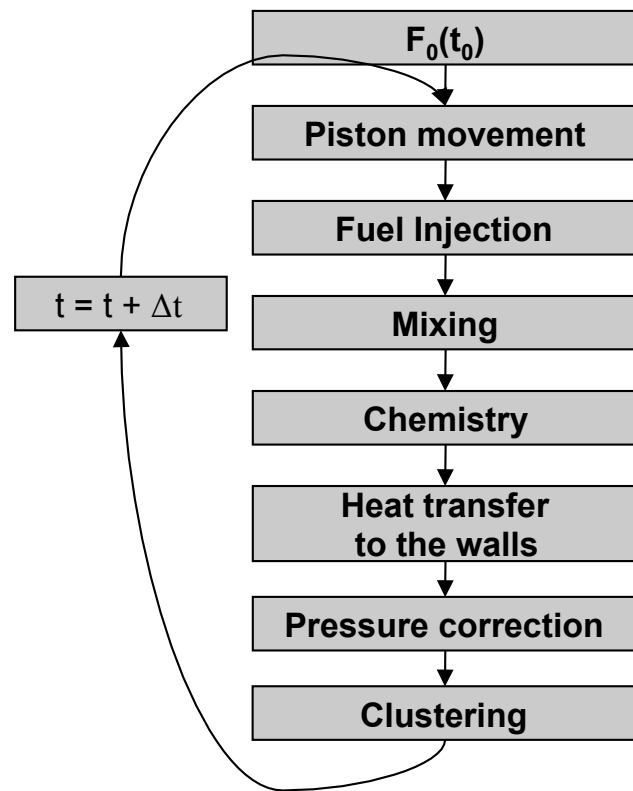
- Our zero-dimensional model is operator-splitted. We solve physical and chemical problems in time steps of about 1 ms.

- This time scale is large compared to that of chemical reactions, so the chemistry needs to be solved by an explicit Euler solver.
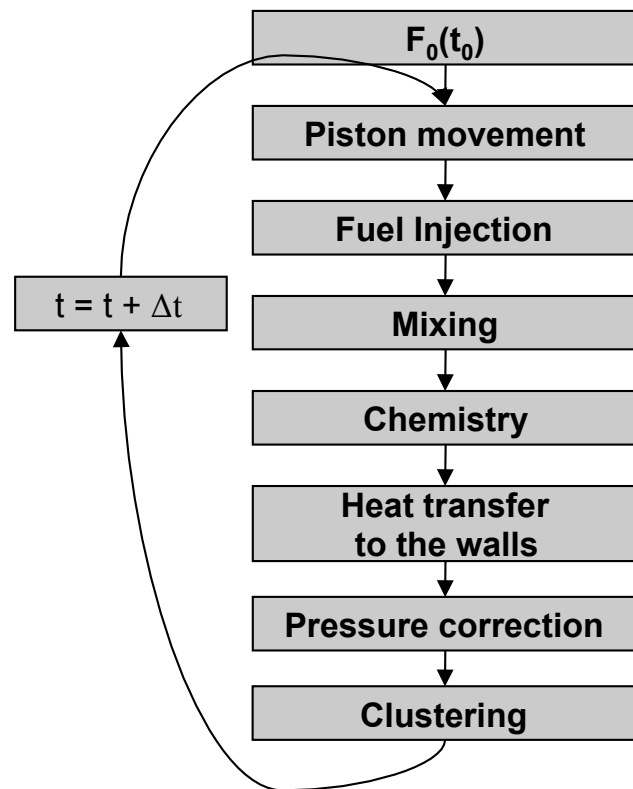
Mathematical applications
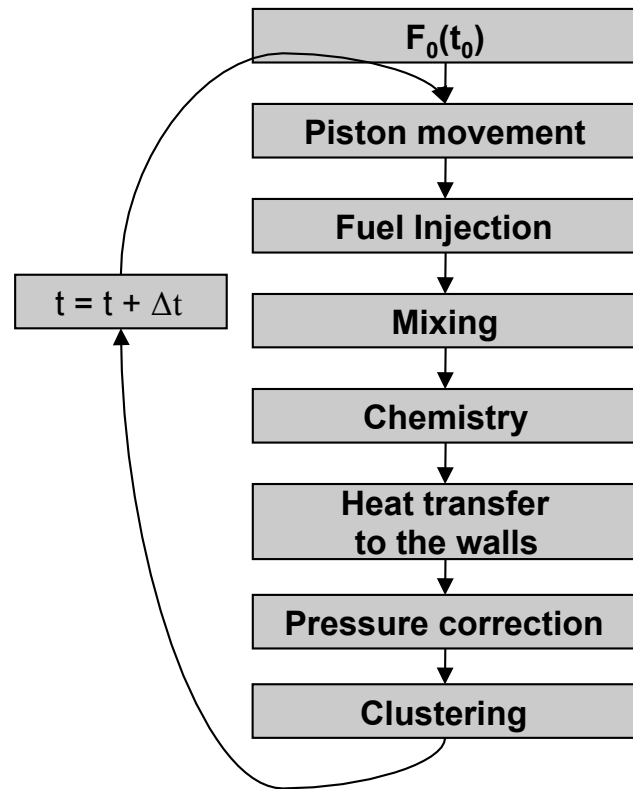
Fuel injection
How to model the injection and vaporization of fuel without having spatial information for the particles?
How to model the increase in mixing that takes place between particles due to the kinetic energy from the gas injection?
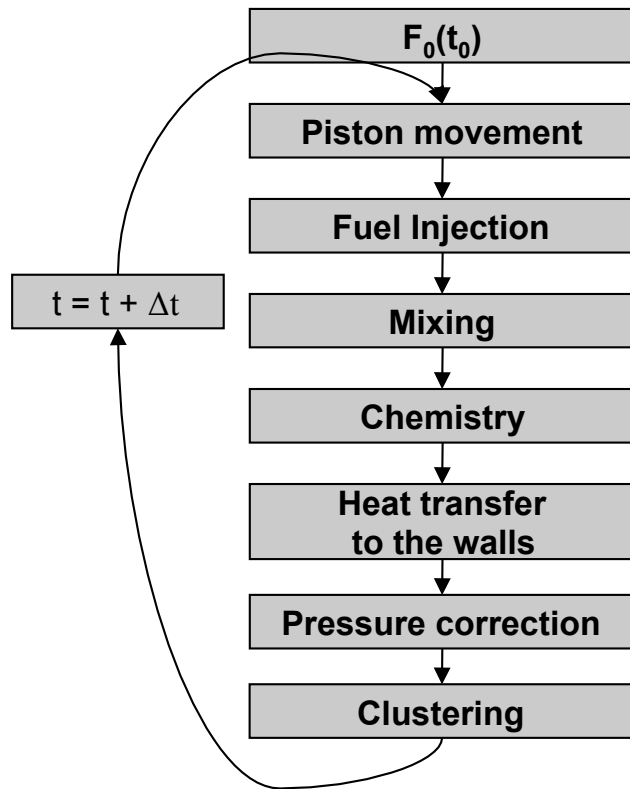
Mathematical applications


```
F_0(t_0)
   |
   v
Piston movement
   |
   v
Fuel Injection
   |
   v
Mixing          <----
   |
   v
Chemistry
   |
   v
Heat transfer
to the walls
   |
   v
Pressure correction
   |
   v
Clustering

t = t + Δt
```

Mixing
There are several models to take into account the random interaction between particles, but they all presume that all parts of the gas are mixing equally fast. Can this be solved by transporting kinetic energy for the particles?
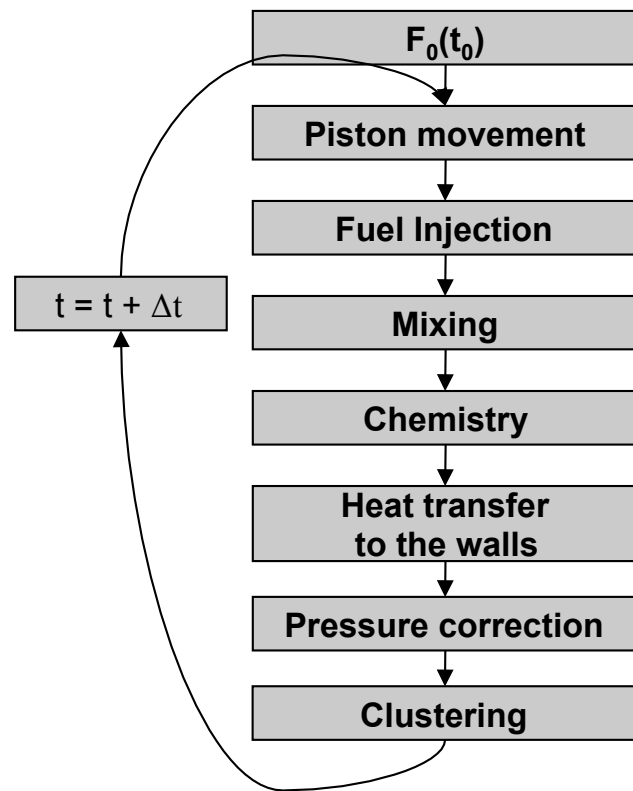
Mathematical applications

Chemistry
The chemistry calculations are significantly more time-consuming than the rest of the simulation. Improving the solver efficiency is always a priority!

Mathematical applications

Clustering
After each time steps, similar particles can be clustered together to improve calculation time for the following step. We are currently looking for someone with expertise in binary trees to help us set up a k-d tree of these particles.

Growing up

- Growing up is generally <u>SCARY</u>. Even more so for mathematicians and scientists.

- Many of you probably know very little about what you want to do in life. Yet if you look around, you will find one thing that fascinates you. The sooner you find this thing, the easier.

- You have the opportunity to write two thesis projects. Use it! Try to do at least one of them somewhere you wouldn't normally think of.

The employer's perspective

- Most potential employers will know absolutely nothing about degrees from the Science Faculty. Employing someone under these conditions can be a huge gamble.

- It's infinitely easier to enter a company as a thesis worker, as an intern, or through a project employment. Get in touch with companies that you are interested in. Tell them what you can do, and ask them if there is a particular problem where your expertise can be used.

- The broader education you have, the better! It's good to have at least some courses in physics, chemistry or biology. Or even engineering! The employer will assume that you are completely clueless regarding anything that isn't in your LADOK document.

- Make sure to learn at least one or two programming languages.

Shameless promoting

- Loge likes scientists and mathematicians. We're always looking for thesis projects, and sometimes for interns.

- We have a long history of good thesis projects, and try to catch the best students either as full-time employees, or through part-time projects beside their studies.

- Above everything else, we are currently desperate to find someone who is interested in data visualization, and who is familiar with Java.