# PKF on 1D chemical transport model

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**Abstract**

This notebook illustrates the use of sympkf to build and handle the PKF dynamics associated with the transport of two chemical species over a 1D domain, and in the case of a periodic chemical reaction. Hence, the dynamics reads as

$$\left\{\begin{array}{c}\partial_t A + u\partial_x A = B\\ \partial_t B + u\partial_x B = -A\end{array}\right.$$

where $A$ and $B$ are functions of $t, x$, and $u(x)$ is a stationnary wind.

Thanks to the splitting strategy, the PKF is first applied in 0D on the periodic reaction, than on the full dynamics.

## 1 Definition of the 1D multivariate dynamics

[1]:
```
import sympy
sympy.init_printing()
```

**Definition of the dynamics from sympy tools**

[2]:
```
from sympy import Function, Derivative, Eq, symbols
from sympkf import SymbolicPKF, t
```

[3]:
```
x = symbols('x')
u = Function('u')(x)
A = Function('A')(t,x)
B = Function('B')(t,x)
```

## 2 0D periodic chemical reaction

[4]:
```
# definition of the dynamics
dynamics = [Eq(Derivative(A,t), B), Eq(Derivative(B,t),-A)]
dynamics
```

[4]: $$\left[ \frac{\partial}{\partial t} A(t,x) = B(t,x),\ \ \frac{\partial}{\partial t} B(t,x) = -A(t,x) \right]$$

[5]:
```
pkf_dynamics = SymbolicPKF(dynamics)
```

[6]:
```
for equation in pkf_dynamics.in_metric:
    #display(equation.subs(pkf_dynamics.internal_closure))
    display(equation)
```

$$\frac{\partial}{\partial t} A(t,x) = B(t,x)$$

$$\frac{\partial}{\partial t} B(t,x) = -A(t,x)$$

$$\frac{\partial}{\partial t} \mathrm{V_A}(t,x) = 2\,\mathrm{V_{AB}}(t,x)$$

$$\frac{\partial}{\partial t} \mathrm{V_B}(t,x) = -2\,\mathrm{V_{AB}}(t,x)$$

$$\frac{\partial}{\partial t} \mathrm{V_{AB}}(t,x) = -\mathrm{V_A}(t,x) + \mathrm{V_B}(t,x)$$

$$\frac{\partial}{\partial t} \mathrm{g_{A,xx}}(t,x) = -\frac{2\,\mathrm{V_{AB}}(t,x)\,\mathrm{g_{A,xx}}(t,x)}{\mathrm{V_A}(t,x)} + \frac{2\sqrt{\mathrm{V_B}(t,x)}\,\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V_A}(t,x)}} + \frac{\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)}{\sqrt{\mathrm{V_A}(t,x)}\sqrt{\mathrm{V_B}(t,x)}} - \frac{\sqrt{\mathrm{V_B}(t,x)}\,\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)}{\mathrm{V_A}^{\frac{3}{2}}(t,x)}$$

$$\frac{\partial}{\partial t} \mathrm{g_{B,xx}}(t,x) = \frac{2\,\mathrm{V_{AB}}(t,x)\,\mathrm{g_{B,xx}}(t,x)}{\mathrm{V_B}(t,x)} - \frac{2\sqrt{\mathrm{V_A}(t,x)}\,\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V_B}(t,x)}} + \frac{\sqrt{\mathrm{V_A}(t,x)}\,\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)}{\mathrm{V_B}^{\frac{3}{2}}(t,x)} - \frac{\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)}{\sqrt{\mathrm{V_A}(t,x)}\sqrt{\mathrm{V_B}(t,x)}}$$

## 3 1D transport of a periodic chemical reaction

[7]:
```
# Definition of the dynamics
dynamics = [Eq(Derivative(A,t),-u*Derivative(A,x)+ B), Eq(Derivative(B,t),␣
↪-u*Derivative(B,x)-A)]
dynamics
```

[7]: $$\left[ \frac{\partial}{\partial t} A(t,x) = B(t,x) - u(x)\frac{\partial}{\partial x}A(t,x),\ \ \frac{\partial}{\partial t} B(t,x) = -A(t,x) - u(x)\frac{\partial}{\partial x}B(t,x) \right]$$

[8]:
```python
pkf_dynamics = SymbolicPKF(dynamics)
```

[9]:
```python
for equation in pkf_dynamics.in_metric:
    #display(equation.subs(pkf_dynamics.internal_closure))
    display(equation)
```

$$\frac{\partial}{\partial t}A(t,x) = B(t,x) - u(x)\frac{\partial}{\partial x}A(t,x)$$

$$\frac{\partial}{\partial t}B(t,x) = -A(t,x) - u(x)\frac{\partial}{\partial x}B(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V_A}(t,x) = 2\,\mathrm{V_{AB}}(t,x) - u(x)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V_B}(t,x) = -2\,\mathrm{V_{AB}}(t,x) - u(x)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V_{AB}}(t,x) = -\frac{\mathrm{V_{AB}}(t,x)u(x)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)}{2\,\mathrm{V_B}(t,x)} - \frac{\mathrm{V_{AB}}(t,x)u(x)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)}{2\,\mathrm{V_A}(t,x)} - u(x)\sqrt{\mathrm{V_A}(t,x)}\sqrt{\mathrm{V_B}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right) - u(x)\sqrt{\mathrm{V_A}(t,x)}\sqrt{\mathrm{V_B}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right) - \mathrm{V_A}(t,x) + \mathrm{V_B}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{g_{A,xx}}(t,x) = -\frac{2\,\mathrm{V_{AB}}(t,x)\,\mathrm{g_{A,xx}}(t,x)}{\mathrm{V_A}(t,x)} - u(x)\frac{\partial}{\partial x}\mathrm{g_{A,xx}}(t,x) - 2\,\mathrm{g_{A,xx}}(t,x)\frac{d}{dx}u(x) + \frac{2\sqrt{\mathrm{V_B}(t,x)}\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V_A}(t,x)}} + \frac{\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)}{\sqrt{\mathrm{V_A}(t,x)}\sqrt{\mathrm{V_B}(t,x)}} - \frac{\sqrt{\mathrm{V_B}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)}{\mathrm{V_A}^{\frac{3}{2}}(t,x)}$$

$$\frac{\partial}{\partial t}\mathrm{g_{B,xx}}(t,x) = \frac{2\,\mathrm{V_{AB}}(t,x)\,\mathrm{g_{B,xx}}(t,x)}{\mathrm{V_B}(t,x)} - u(x)\frac{\partial}{\partial x}\mathrm{g_{B,xx}}(t,x) - \frac{2\sqrt{\mathrm{V_A}(t,x)}\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V_B}(t,x)}} + \frac{\sqrt{\mathrm{V_A}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)}{\mathrm{V_B}^{\frac{3}{2}}(t,x)} - 2\,\mathrm{g_{B,xx}}(t,x)\frac{d}{dx}u(x) - \frac{\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)}{\sqrt{\mathrm{V_A}(t,x)}\sqrt{\mathrm{V_B}(t,x)}}$$

[10]:
```python
for equation in pkf_dynamics.in_metric:
    display(equation.subs(pkf_dynamics.internal_closure))
```

$$\frac{\partial}{\partial t}A(t,x) = B(t,x) - u(x)\frac{\partial}{\partial x}A(t,x)$$

$$\frac{\partial}{\partial t}B(t,x) = -A(t,x) - u(x)\frac{\partial}{\partial x}B(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V_A}(t,x) = 2\,\mathrm{V_{AB}}(t,x) - u(x)\frac{\partial}{\partial x}\mathrm{V_A}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V_B}(t,x) = -2\,\mathrm{V_{AB}}(t,x) - u(x)\frac{\partial}{\partial x}\mathrm{V_B}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V}_{\mathrm{AB}}(t,x) = -\frac{\mathrm{V}_{\mathrm{AB}}(t,x)u(x)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(t,x)}{2\,\mathrm{V}_{\mathrm{B}}(t,x)} - \frac{\mathrm{V}_{\mathrm{AB}}(t,x)u(x)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}(t,x)}{2\,\mathrm{V}_{\mathrm{A}}(t,x)} - u(x)\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right) - u(x)\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right) - \mathrm{V}_{\mathrm{A}}(t,x) + \mathrm{V}_{\mathrm{B}}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{g}_{\mathrm{A,xx}}(t,x) = -\frac{2\,\mathrm{V}_{\mathrm{AB}}(t,x)\,\mathrm{g}_{\mathrm{A,xx}}(t,x)}{\mathrm{V}_{\mathrm{A}}(t,x)} - u(x)\frac{\partial}{\partial x}\mathrm{g}_{\mathrm{A,xx}}(t,x) - 2\,\mathrm{g}_{\mathrm{A,xx}}(t,x)\frac{d}{dx}u(x) + \frac{2\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}} + \frac{\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(t,x)}{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}} - \frac{\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}(t,x)}{\mathrm{V}_{\mathrm{A}}^{\frac{3}{2}}(t,x)}$$

$$\frac{\partial}{\partial t}\mathrm{g}_{\mathrm{B,xx}}(t,x) = \frac{2\,\mathrm{V}_{\mathrm{AB}}(t,x)\,\mathrm{g}_{\mathrm{B,xx}}(t,x)}{\mathrm{V}_{\mathrm{B}}(t,x)} - u(x)\frac{\partial}{\partial x}\mathrm{g}_{\mathrm{B,xx}}(t,x) - \frac{2\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}} + \frac{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(t,x)}{\mathrm{V}_{\mathrm{B}}^{\frac{3}{2}}(t,x)} - 2\,\mathrm{g}_{\mathrm{B,xx}}(t,x)\frac{d}{dx}u(x) - \frac{\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}(t,x)}{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}}$$

[11]:
```
for equation in pkf_dynamics.in_aspect:    display(equation)
```

$$\frac{\partial}{\partial t}A(t,x) = B(t,x) - u(x)\frac{\partial}{\partial x}A(t,x)$$

$$\frac{\partial}{\partial t}B(t,x) = -A(t,x) - u(x)\frac{\partial}{\partial x}B(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V}_{\mathrm{A}}(t,x) = 2\,\mathrm{V}_{\mathrm{AB}}(t,x) - u(x)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V}_{\mathrm{B}}(t,x) = -2\,\mathrm{V}_{\mathrm{AB}}(t,x) - u(x)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{V}_{\mathrm{AB}}(t,x) = -\frac{\mathrm{V}_{\mathrm{AB}}(t,x)u(x)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(t,x)}{2\,\mathrm{V}_{\mathrm{B}}(t,x)} - \frac{\mathrm{V}_{\mathrm{AB}}(t,x)u(x)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}(t,x)}{2\,\mathrm{V}_{\mathrm{A}}(t,x)} - u(x)\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right) - u(x)\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right) - \mathrm{V}_{\mathrm{A}}(t,x) + \mathrm{V}_{\mathrm{B}}(t,x)$$

$$\frac{\partial}{\partial t}\mathrm{s}_{\mathrm{A,xx}}(t,x) = \frac{2\,\mathrm{V}_{\mathrm{AB}}(t,x)\,\mathrm{s}_{\mathrm{A,xx}}(t,x)}{\mathrm{V}_{\mathrm{A}}(t,x)} - u(x)\frac{\partial}{\partial x}\mathrm{s}_{\mathrm{A,xx}}(t,x) + 2\,\mathrm{s}_{\mathrm{A,xx}}(t,x)\frac{d}{dx}u(x) - \frac{2\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\,\mathrm{s}_{\mathrm{A,xx}}^{2}(t,x)\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}} - \frac{\mathrm{s}_{\mathrm{A,xx}}^{2}(t,x)\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(t,x)}{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}} + \frac{\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}\,\mathrm{s}_{\mathrm{A,xx}}^{2}(t,x)\mathbb{E}\left(\varepsilon_{\mathrm{B}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}(t,x}{\mathrm{V}_{\mathrm{A}}^{\frac{3}{2}}(t,x)}$$

$$\frac{\partial}{\partial t}\mathrm{s}_{\mathrm{B,xx}}(t,x) = -\frac{2\,\mathrm{V}_{\mathrm{AB}}(t,x)\,\mathrm{s}_{\mathrm{B,xx}}(t,x)}{\mathrm{V}_{\mathrm{B}}(t,x)} - u(x)\frac{\partial}{\partial x}\mathrm{s}_{\mathrm{B,xx}}(t,x) + \frac{2\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\,\mathrm{s}_{\mathrm{B,xx}}^{2}(t,x)\mathbb{E}\left(\frac{\partial}{\partial x}\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)}{\sqrt{\mathrm{V}_{\mathrm{B}}(t,x)}} - \frac{\sqrt{\mathrm{V}_{\mathrm{A}}(t,x)}\,\mathrm{s}_{\mathrm{B,xx}}^{2}(t,x)\mathbb{E}\left(\varepsilon_{\mathrm{A}}(t,x,\omega)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}(t,x,\omega)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{B}}(}{\mathrm{V}_{\mathrm{B}}^{\frac{3}{2}}(t,x)}$$

$$2\,\mathrm{s}_{\mathrm{B,xx}}\left(t,x\right)\frac{d}{dx}u(x)+\frac{{\mathrm{s}_{\mathrm{B,xx}}}^{2}\left(t,x\right)\mathbb{E}\left(\varepsilon_{\mathrm{A}}\left(t,x,\omega\right)\frac{\partial}{\partial x}\varepsilon_{\mathrm{B}}\left(t,x,\omega\right)\right)\frac{\partial}{\partial x}\mathrm{V}_{\mathrm{A}}\left(t,x\right)}{\sqrt{\mathrm{V}_{\mathrm{A}}\left(t,x\right)}\sqrt{\mathrm{V}_{\mathrm{B}}\left(t,x\right)}}$$