Doc: continuous models

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$$m(\boldsymbol{x})\frac{\partial^2}{\partial t^2}\theta(\boldsymbol{x},t) + d(\boldsymbol{x})\frac{\partial}{\partial t}\theta(\boldsymbol{x},t) = p(\boldsymbol{x},t) + \boldsymbol{\nabla}\cdot\left[\boldsymbol{b}(\boldsymbol{x})\circ\boldsymbol{\nabla}\theta(\boldsymbol{x},t)\right]\,, \tag{1}$$

Discretizing in time and space, updated state is computed as

$$\begin{aligned}\theta_{i,j}(t+\Delta t) = &\left[2\chi_{ij} - \frac{\Delta t^2 m_{ij}^{-1}\chi_{ij}}{\Delta x^2}\Big(b_{i,j|i+1,j} + b_{i-1,j|i,j} + b_{i,j|i,j+1} + b_{i,j-1|i,j}\Big)\right]\theta_{i,j}(t)\\ &- \left[1 - \frac{\gamma_{i,j}\Delta t}{2}\right]\chi_{ij}\theta_{i,j}(t-\Delta t) + \frac{\Delta t^2\chi_{i,j}m_{ij}^{-1}}{\Delta x^2}\Big[b_{i-1,j|i,j}\theta_{i-1,j}(t) + b_{i,j|i+1,j}\theta_{i+1,j}(t)\\ &+ b_{i,j-1|i,j}\theta_{i,j-1}(t) + b_{i,j|i,j+1}\theta_{i,j+1}(t)\Big] + \Delta t^2\chi_{ij}m_{ij}^{-1}p_{i,j}\,,\end{aligned} \tag{2}$$

where $\chi_{i,j} = \left[1 + \frac{\gamma_{i,j}\Delta t}{2}\right]^{-1}$ and $\gamma_{i,j} = d_{i,j}/m_{i,j}$.

The previous equation follows from

$$\boldsymbol{\nabla}\cdot\left[\boldsymbol{b}(\boldsymbol{x})\circ\boldsymbol{\nabla}\theta(\boldsymbol{x},t)\right] = \partial_x b_x\partial_x\theta + b_x\partial_x^2\theta + \partial_y b_y\partial_y\theta + b_y\partial_y^2\theta\,, \tag{3}$$

where

$$b_x(\boldsymbol{x}) \approx \frac{b^x_{i,j-1} + b^x_{i,j}}{2}\,, \tag{4}$$

$$\partial_x b_x \approx \frac{b^x_{i,j} - b^x_{i,j-1}}{\Delta x}\,, \tag{5}$$

$$\partial_x\theta \approx \frac{\theta_{i+1,j} - \theta_{i-1,j}}{2\Delta x}\,, \tag{6}$$

$$\partial_x^2\theta \approx \frac{\theta_{i-1,j} - 2\theta_{i,j} + \theta_{i+1,j}}{\Delta x^2}\,, \tag{7}$$

So, finally

$$\partial_x b_x\partial_x\theta + b_x\partial_x^2\theta + \partial_y b_y\partial_y\theta + b_y\partial_y^2\theta \approx \tag{8}$$

$$\frac{b^x_{i,j-1}\theta_{i,j-1} + b^x_{i,j}\theta_{i,j+1} + b^y_{i-1,j}\theta_{i-1,j} + b^y_{i,j}\theta_{i+1,j} - \overbrace{\left(b^x_{i,j-1} + b^x_{i,j} + b^x_{i-1,j} + b^y_{i,j}\right)}^{=\beta}\theta_{i,j}}{\Delta x^2}\,, \tag{9}$$

I. STEADY STATE

Steady state is obtained iteratively as

$$\theta^{(n+1)}_{i,j} = \frac{\Delta x^2\,p_{i,j} + b^y_{i,j}\theta^{(n)}_{i-1,j} + b^y_{i,j}\theta^{(n)}_{i+1,j} + b^x_{i,j-1}\theta^{(n)}_{i,j-1} + b^x_{i,j}\theta^{(n)}_{i,j+1}}{b^y_{i,j} + b^y_{i-1,j} + b^x_{i,j} + b^x_{i,j-1}} \tag{10}$$

II. BOUNDARY CONDITIONS

$$\int\limits_{\partial\Omega} b(\boldsymbol{x})\circ\nabla\theta(\boldsymbol{x},t)\cdot\boldsymbol{n}\,\mathrm{d}\boldsymbol{x} = 0, \tag{11}$$

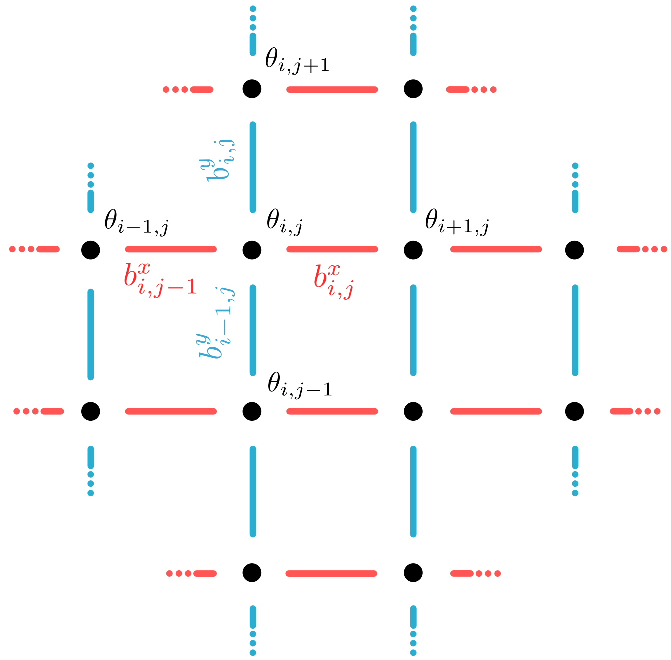

FIG. 1. How it is implemented.

which is trivially true, if

$$n_x b_x \partial_x \theta(\boldsymbol{x}) + n_y b_y \partial_y \theta(\boldsymbol{x}) = 0\,, \ \forall t \text{ and } \boldsymbol{x} \in \partial\Omega\,, \tag{12}$$

For the moment, lets assume in 1D and treating the case $n_x = -1$.

$$b_x(x)\partial_x\theta(x) = 0 \tag{13}$$

$$b_x(x+\Delta x)\theta(x+\Delta x) = b_x(x)\theta(x) + \Big(\partial_x b_x(x)\theta(x) + \cancelto{0,\ \text{b.c.}}{b_x(x)\partial_x\theta(x)}\Big)\Delta x + (\cdots)\Delta x^2/2 + O(\Delta x^3) \tag{14}$$

$$b_x(x+2\Delta x)\theta(x+2\Delta x) = b_x(x)\theta(x) + \Big(\partial_x b_x(x)\theta(x) + \cancelto{0,\ \text{b.c.}}{b_x(x)\partial_x\theta(x)}\Big)2\Delta x + 2(\cdots)\Delta x^2 + O(\Delta x^3) \tag{15}$$

(From the 1st equation, we get

$$\theta_{i,j} = \frac{(b^x_{i,j} + b^x_{i,j+1})\theta_{i,j+1}}{3b^x_{i,j} - b^x_{i,j-1}} + O(\Delta x^2) \tag{16}$$

which is not exactly what was implemented. It might be enough to change that...) Summing four times the 1st equation with minus the second, one gets

$$\theta(x) = \frac{4b_x(x+\Delta x)\theta(x+\Delta x) - b_x(x+2\Delta x)\theta(x+2\Delta x)}{3b_x(x) + 2\Delta x \partial_x b_x} + O(\Delta x^3) \tag{17}$$

Converting this expression with Eqs. 4-7, we get

$$\theta_{i,j} = \frac{4(b^x_{i,j} + b^x_{i,j+1})\theta_{i,j+1} - (b^x_{i,j+1} + b^x_{i,j+2})\theta_{i,j+2}}{3(b^x_{i,j-1} + b^x_{i,j}) + 4(b^x_{i,j} - b^x_{i,j-1})} \tag{18}$$

What to do? Set $b^x_{i,j-1}$ to 0 or to $b^x_{i,j}$!? (My opinion is that we should set it to 0. I agree with that.)

Analogously we obtain for $n_x = 1$ we obtain by changing $\Delta x \to -\Delta x$

$$\theta_{i,j} = \frac{4(b^x_{i,j-2} + b^x_{i,j-1})\theta_{i,j-1} - (b^x_{i,j-3} + b^x_{i,j-2})\theta_{i,j-2}}{3(b^x_{i,j-1} + b^x_{i,j}) - 4(b^x_{i,j} - b^x_{i,j-1})} \tag{19}$$

In this case we should set $b^x_{i,j} = 0$.

For the corners we can use ($n_x = -1$, $n_y = -1$)

$$\begin{aligned} b_x(x+\Delta,y)\theta(x+\Delta,y) + b_y(x,y+\Delta)\theta(x,y+\Delta) &= (b_x(x,y)+b_y(x,y))\theta(x,y) + \\ &\quad 0,\, b.c. \\ \big(b_x(x,y)\partial_x\theta(x,y) + b_y(x,y)\partial_y\theta(x,y) &+ b_x(x,y)\partial_y\theta(x,y) + b_y(x,y)\partial_x\theta(x,y)\big)\Delta + (\dots)\Delta^2/2 + \mathcal{O}(\Delta^3), \end{aligned} \tag{20}$$

$$\begin{aligned} b_x(x+2\Delta,y)\theta(x+2\Delta,y) + b_y(x,y+2\Delta)\theta(x,y+2\Delta) &= (b_x(x,y)+b_y(x,y))\theta(x,y) + \\ &\quad 0,\, b.c. \\ 2\big(b_x(x,y)\partial_x\theta(x,y) + b_y(x,y)\partial_y\theta(x,y) &+ b_x(x,y)\partial_y\theta(x,y) + b_y(x,y)\partial_x\theta(x,y)\big)\Delta + 2(\dots)\Delta^2 + \mathcal{O}(\Delta^3) \end{aligned} \tag{21}$$

This means for the corners the $\theta_{i,j}$ is given by the sum of (18) and its y equivalent.

Now treating the full case (setting the b outside the grid to 0), lets first define

$$\eta_\pm(x) = 1 \pm x/2 - x^2/2\,, \tag{22}$$

Note that $\eta_+(-1) = 0$, $\eta_+(0) = 1$, $\eta_+(1) = 1$, $\eta_-(-1) = 1$, $\eta_-(0) = 1$ and $\eta_-(1) = 0$.

$$\beta = \eta_+(n_x)b^x_{i,j-1} + \eta_-(n_x)b^x_{i,j} + \eta_+(n_y)b^y_{i,j-1} + \eta_-(n_y)b^y_{i,j}\,, \tag{23}$$

III. VECTORIZATION

The different quantities are flattened, as follows

$$\theta_{i,j} \to \tilde\theta_k\,, \tag{24}$$

with $k = N_y(i-1)+j$. With this change in the indexing, the indices of neighbouring nodes become

$$i-1, j \to k-1\,, \tag{25}$$

$$i+1, j \to k+1\,, \tag{26}$$

$$i, j-1 \to k-N_y\,, \tag{27}$$

$$i, j+1 \to k+N_y\,, \tag{28}$$

$$\xi_{i,j}(\boldsymbol{\theta}) = -\big(b^x_{i,j-1} + b^x_{i,j} + b^y_{i-1,j} + b^y_{i,j}\big)\theta_{i,j} + b^x_{i,j-1}\theta_{i,j-1} + b^x_{i,j}\theta_{i,j+1} + b^y_{i-1,j}\theta_{i-1,j} + b^y_{i,j}\theta_{i+1,j}\,, \tag{29}$$

The function $\boldsymbol{\xi}(\boldsymbol{\theta})$ can be represented as a matrix acting on the flattened $\tilde{\boldsymbol{\theta}}$,

$$\boldsymbol{\xi}(\boldsymbol{\theta}) = \boldsymbol{\Xi}\,\tilde{\boldsymbol{\theta}}\,. \tag{30}$$

The elements of $\boldsymbol{\Xi}$ read

$$\Xi_{kl} = -\big(\tilde b^x_k + \tilde b^x_{k-N_y} + \tilde b^y_k + \tilde b^y_{k-1}\big)\delta_{k,l} + \tilde b^x_{k-N_y}\delta_{k-N_y,l} + \tilde b^x_k\delta_{k+N_y,l} + \tilde b^y_{k-1}\delta_{k-1,l} + \tilde b^y_k\delta_{k+1,l}\,, \tag{31}$$

with $\delta_{\cdot,\cdot}$ is the Kronecker product.

IV. CRANK–NICOLSON

$$\theta_{i,j}(t+\Delta t) - \frac{\Delta t}{2}\,\omega_{i,j}(t+\Delta t) = \theta_{i,j}(t) + \frac{\Delta t}{2}\,\omega_{i,j}(t)\,, \tag{32}$$

$$\Big(1+\frac{\gamma_{i,j}\Delta t}{2}\Big)\omega_{i,j}(t+\Delta t) - \frac{\Delta t}{2}\xi\big(\theta_{i,j}(t+\Delta t)\big) = \Big(1-\frac{\gamma_{i,j}\Delta t}{2}\Big)\omega_{i,j}(t) + \frac{\Delta t}{2}\xi\big(\theta_{i,j}(t)\big) + (2m_{i,j})^{-1}\Big[p_{i,j}(t+\Delta t) + p_{i,j}(t)\Big]\,, \tag{33}$$

$$\underbrace{\begin{bmatrix} \mathbb{1} & -\frac{\Delta t}{2}\mathbb{1} \\ -\frac{\Delta t}{2\Delta x^2}\boldsymbol{M}^{-1}\boldsymbol{\Xi} & \mathbb{1}+\frac{\Delta t}{2}\boldsymbol{\Gamma} \end{bmatrix}}_{=\boldsymbol{A}}\boldsymbol{x}(t+\Delta t) = \underbrace{\begin{bmatrix} \mathbb{1} & \frac{\Delta t}{2}\mathbb{1} \\ \frac{\Delta t}{2\Delta x^2}\boldsymbol{M}^{-1}\boldsymbol{\Xi} & \mathbb{1}-\frac{\Delta t}{2}\boldsymbol{\Gamma} \end{bmatrix}}_{=\boldsymbol{B}}\boldsymbol{x}(t) + \underbrace{\begin{bmatrix} \mathbb{0} \\ \boldsymbol{\pi} \end{bmatrix}}_{=\boldsymbol{C}}, \tag{34}$$

with $\boldsymbol{x}^\top = [\tilde{\boldsymbol{\theta}}^\top\ \tilde{\boldsymbol{\omega}}^\top]$.