Seminar Computational Mathematics

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1 AMB+ Model

The AMB+ Model is given by:

$$\begin{aligned}
\partial_t\phi &= -\nabla\cdot(J+\sqrt{2DM}\Lambda)\\
&= -\nabla\cdot(M(-\nabla\mu_\lambda+\zeta(\nabla^2\phi)\nabla\phi)+\sqrt{2DM}\Lambda)\\
&= -\nabla\cdot(M(-\nabla(\frac{\partial F}{\partial\phi}+\lambda|\nabla\phi|^2)+\zeta(\nabla^2\phi)\nabla\phi)+\sqrt{2DM}\Lambda)
\end{aligned}$$

Where we have F and its functional derivative $\frac{\partial F}{\partial\phi}$ given by

$$\begin{aligned}
F &= \int \frac{a}{2}\phi^2+\frac{b}{4}\phi^4+\frac{\epsilon}{2}|\nabla\phi|^2 dr\\
\frac{\partial F}{\partial\phi} &= a\phi+b\phi^3-\epsilon\nabla^2\phi
\end{aligned}$$

The parameters $a, b, \lambda, \epsilon, \zeta, M, D \in \mathbb{R}$ and Λ is standard normal gaussian noise.
Overall we have:

$$\begin{aligned}
\partial_t\phi &= -\nabla\cdot(M(-\nabla(a\phi+b\phi^3-\epsilon\nabla^2\phi+\lambda|\nabla\phi|^2)+\zeta(\nabla^2\phi)\nabla\phi)+\sqrt{2DM}\Lambda)\\
&= aM\nabla^2\phi+bM\nabla^2(\phi^3)-\epsilon M\nabla^4\phi+\lambda M\nabla^2|\nabla\phi|^2-\zeta M\nabla\cdot(\nabla^2\phi)\nabla\phi-\nabla\cdot\sqrt{2DM}\Lambda)\\
&=: L(\phi)+N(\phi)-\nabla\cdot\sqrt{2DM}\Lambda
\end{aligned}$$

Defining

$$\begin{aligned}
L(\phi) &= aM\nabla^2\phi-\epsilon M\nabla^4\phi\\
N(\phi) &= bM\nabla^2(\phi^3)+\lambda M\nabla^2|\nabla\phi|^2-\zeta M\nabla\cdot(\nabla^2\phi)\nabla\phi
\end{aligned}$$

2 Pseudospectral Fourier Method applied on AMB+

We can now use the pseudospectral Fourier method as follows:

$$\begin{aligned}
\partial_t \widehat{\phi} &= \widehat{L} \cdot \widehat{\phi} + \widehat{N(\phi)} - \sqrt{2DM} i(\vec{k} \cdot \widehat{\Lambda}) \\
&= (-aM\vec{k}^2 - \epsilon M\vec{k}^4)\widehat{\phi} + \widehat{N(\phi)} - \sqrt{2DM} i(\vec{k} \cdot \widehat{\Lambda})
\end{aligned}$$

We discretize using a semi-implicit Euler scheme (with scaling for the stochastic part):

$$\begin{aligned}
\widehat{\phi}^{(n+1)} &= \widehat{\phi}^{(n)} + \tau((-aM\vec{k}^2 - \epsilon M\vec{k}^4)\widehat{\phi}^{(n+1)} + \widehat{N(\phi^{(n)})}) - \sqrt{2DM\tau} i(\vec{k} \cdot \widehat{\Lambda}^{(n)}) \\
\implies \widehat{\phi}^{(n+1)} &= \frac{\widehat{\phi}^{(n)} + \tau \widehat{N(\phi^{(n)})} - \sqrt{2DM\tau} i(\vec{k} \cdot \widehat{\Lambda}^{(n)})}{1 - \tau(-\epsilon M\vec{k}^4 - aM\vec{k}^2)}
\end{aligned}$$

Here we can compute the nonlinear term, given $\phi^{(n)}, \nabla\phi^{(n)}, \nabla^2\phi^{(n)}$, as

$$\widehat{N(\phi^{(n)})} = -bM\vec{k}^2 \widehat{{\phi^{(n)}}^3} - \lambda M\vec{k}^2 \widehat{|\nabla\phi^{(n)}|^2} - \zeta M i\vec{k} \cdot \widehat{(\nabla^2\phi^{(n)})\nabla\phi^{(n)}}$$

Substitution into the time-stepping scheme above leads to the overall formula

$$\widehat{\phi}^{(n+1)} = \frac{\widehat{\phi}^{(n)} + \tau(-M\vec{k}^2 \widehat{(b{\phi^{(n)}}^3 + \lambda|\nabla\phi^{(n)}|^2)} - \zeta M i\vec{k} \cdot \widehat{(\nabla^2\phi^{(n)})\nabla\phi^{(n)}}) - \sqrt{2DM\tau} i(\vec{k} \cdot \widehat{\Lambda}^{(n)})}{1 + \tau(\epsilon M\vec{k}^4 + aM\vec{k}^2)}$$

where we compute $\phi^{(n)}, \nabla\phi^{(n)}, \nabla^2\phi^{(n)}$ from $\widehat{\phi}^{(n)}$ by

$$\begin{aligned}
\phi^{(n)} &= \mathcal{F}^{-1}(\widehat{\phi}^{(n)}) \\
\nabla\phi^{(n)} &= \mathcal{F}^{-1}(i\vec{k}\widehat{\phi}^{(n)}) \\
\nabla^2\phi^{(n)} &= \mathcal{F}^{-1}(-\vec{k}^2\widehat{\phi}^{(n)})
\end{aligned}$$

which immediately implies an algorithmic implementation. For a space discretization we also need to scale $\widehat{\Lambda}^{(n)}$ by $(\Delta x \Delta y)^{-\frac{1}{2}}$

3 Algorithm/Implementation

Algorithm 1: Solving AMB+ with Fourier Pseudospectral Method and semi-implicit Euler

Data: $\phi^{(0)} \in \mathbb{R}^d, a, b, \lambda, \epsilon, \zeta, M, D, \tau \in \mathbb{R}, N \in \mathbb{N}$,
Result: $\phi^{(N+1)}$

$\widehat{\phi}^{(0)} \leftarrow FFT(\phi^{(0)})$
Precompute $\vec{k}^2, \vec{k}^4$
`// Time-stepping loop`
for $n = 0, \ldots, N$ **do**
    Compute $\nabla\phi^{(n)}, \nabla^2\phi^{(n)}$ from $\widehat{\phi}^{(n)}$ using iFFT
    Sample random white noise $\Lambda^{(n)}$
    Compute $\widehat{\phi}^{(n+1)}$ as above
    Compute $\phi^{(n+1)}$ from $\widehat{\phi}^{(n+1)}$ using iFFT
end