

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:

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

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

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

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.

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: $\phi^{(N+1)}$

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