On second order in time numerical schemes for the Cahn-Hilliard equation

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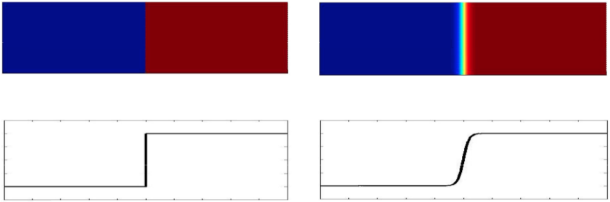

Sharp interface Phase field

- **Sharp-interface** models
  - PDE for each phase + coupled interface conditions
  - Very difficult numerically (interface tracking)
- **Diffuse interface** Phase-field models
  - Phase function with distinct values (for instance +1 and -1) in each phase, with a smooth change in the interface (of width ε).
  - Surface motion depending on the physical energy dissipation.
  - When interface width ε tends to zero, recover a sharp interface model.

Motivation

Design numerical schemes for diffuse-interface phase-field problems:

1. Efficient in time (Linear schemes, adaptive time-step).
2. Suitable to use (standard) Finite Elements (mesh adaptation)
3. Mimic properties of the continuous problem: Dissipative Energy law, maximum principle, small parameter (interface thickness), ...
4. Good finite time and large time accurate (infinite equilibrium states)

Numerical analysis:

1. Large time Energy Stability
2. Unique Solvability of the schemes
3. Convergence of iterative algorithms approximating nonlinear schemes

Application to other energy-based models:

1. Two-phase flows with different densities
2. Vesicle membranes
3. Liquid crystal
4. ...

The **Allen-Cahn** and the **Cahn-Hilliard** models are **gradient flows** for the same **Free Energy** (Liapunov functional):

$$E(\phi) = E_{philic}(\phi) + E_{phobic}(\phi) := \int_\Omega \left(\frac{1}{2} |\nabla \phi|^2 + F(\phi) \right) dx$$

where $F(\phi)$ is a **double-well potential** taking two minimum (stable) values:

$$F(\phi) = \frac{1}{4\varepsilon^2}(\phi^2 - 1)^2$$ at $\phi = \pm 1$ (**Ginzburg-Landau** potential)

- **Allen-Cahn :** $\phi_t + \gamma \dfrac{\delta E}{\delta \phi} = 0$ $\Rightarrow$ Maximum Principle
- **Cahn-Hilliard :** $\phi_t - \nabla \cdot \left(M(\phi) \nabla \dfrac{\delta E}{\delta \phi} \right) = 0 \Rightarrow$ Mass Consevation

where $\dfrac{\delta E}{\delta \phi} = -\Delta \phi + f(\phi)$ with $f(\phi) = F'(\phi)$.

In both cases: $d_t E(\phi(t)) \leq 0$.

Weak formulation: Find (ϕ, w) such that

$$\phi \in L^\infty((0,T);H^1(\Omega)) \quad \text{and} \quad w \in L^2((0,T);H^1(\Omega))$$

satisfying

$$\begin{cases} \langle \phi_t, \overline{w} \rangle + \gamma \Big(\nabla w, \nabla \overline{w} \Big) = 0 & \forall\, \overline{w} \in H^1(\Omega) \\ \Big(\nabla \phi, \nabla \overline{\phi} \Big) + \Big(f(\phi), \overline{\phi} \Big) - \Big(w, \overline{\phi} \Big) = 0 & \forall\, \overline{\phi} \in H^1(\Omega). \end{cases}$$

Energy Law:

$$\frac{d}{dt} E(\phi(t)) + \gamma \int_\Omega |\nabla w|^2 dx = 0.$$

Mathematical Analysis: Abels, Garcke, Grasselli, Miranville, Schimperna, ...
Numerical Analysis: Boyer, Elliot, Feng, Gómez, Hughes, Prohl, ...

Second Order Schemes for the Cahn-Hilliard model

Generic Second order Finite Difference schemes
(Crank-Nicolson for linear terms)

$$\begin{cases} \left(\delta_t\phi^{n+1}, \overline{w}\right) + \gamma\left(\nabla w^{n+\frac{1}{2}}, \nabla\overline{w}\right) = 0 \qquad \forall\, \overline{w} \in H^1(\Omega) \\ \left(\nabla\left(\dfrac{\phi^{n+1}+\phi^n}{2}\right), \nabla\overline{\phi}\right) + \left(f^k(\phi^{n+1}, \phi^n), \overline{\phi}\right) - \left(w^{n+\frac{1}{2}}, \overline{\phi}\right) = 0 \qquad \forall\, \overline{\phi} \end{cases}$$

where $\delta_t\phi^{n+1} = (\phi^{n+1} - \phi^n)/k$ (discrete time derivative).

Discrete Energy Law: Testing by $(\overline{w}, \overline{\phi}) = (w^{n+\frac{1}{2}}, \delta_t\phi^{n+1})$

$$\delta_t E(\phi^{n+1}) + \gamma\|\nabla w^{n+\frac{1}{2}}\|^2_{L^2} + \xcancel{ND_{philic}(\phi^{n+1}, \phi^n)} + ND_{phobic}(\phi^{n+1}, \phi^n) = 0,$$

where

$$ND_{phobic}(\phi^{n+1}, \phi^n) := \left(f^k(\phi^{n+1}, \phi^n), \delta_t\phi^{n+1}\right) - \delta_t\left(\int_\Omega F(\phi^{n+1})\right)$$

Definition

Numerical schemes are energy-stable if

$$\delta_t E(\phi^{n+1}) + \gamma \int_\Omega |\nabla w^{n+\frac{1}{2}}|^2 \leq 0, \quad \forall\, n.$$

In particular, the discrete energy decreases,

$$E(\phi^{n+1}) \leq E(\phi^n), \quad \forall\, n.$$

Eyre's decomposition

[Eyre]
Splitting the potential term

$F(\phi) = F_c(\phi)+F_e(\phi)$ with $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave)

Taking implicitly the convex term and explicitly the non-convex one, i.e.

$$f^k(\phi^{n+1}, \phi^n) = f_c(\phi^{n+1}) + f_e(\phi^n) = \frac{1}{\varepsilon^2}((\phi^{n+1})^3 - \phi^n),$$

Properties:

- First order accurate
- Nonlinear scheme
- Unconditionally unique solvable
- Unconditionally energy-stable

Midpoint approximation of the potential term **[Elliot], [Du], [Lin],...**

$$f^k(\phi^{n+1},\phi^n) = \frac{F(\phi^{n+1}) - F(\phi^n)}{\phi^{n+1} - \phi^n}$$

Then

$$ND_{phobic}(\phi^{n+1},\phi^n) = 0 \quad \Rightarrow \quad \delta_t E(\phi^{n+1}) + \gamma \|\nabla w^{n+\frac{1}{2}}\|^2_{L^2} = 0$$

Properties:

- Second order accurate
- Nonlinear scheme
- Conditionally unique solvable ($k < \varepsilon^4/\gamma$)
- Unconditionally energy-stable

Theorem

- *Solvability hypothesis*

$$k < \frac{4\varepsilon^4}{\gamma}$$

- *Convergence hypothesis*

$$\frac{k^{1/2}}{\varepsilon^4} < C \quad \textit{and} \quad \lim_{(k,h)\to 0} \frac{k}{h^2} = 0.$$

[Wang et al.]
Splitting the potential term $F(\phi) = F_c(\phi) + F_e(\phi)$ with $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave) Taking **MP** for the convex term and **BDF2** for the non-convex:

$$f^k(\phi^{n+1}, \phi^n, \phi^{n-1}) = \frac{F_c(\phi^{n+1}) - F_c(\phi^n)}{\phi^{n+1} - \phi^n} + \frac{1}{2}\Big(3f_e(\phi^n) - f_e(\phi^{n-1})\Big).$$

Properties:

- Second order accurate
- Nonlinear scheme
- Unconditionally unique solvable
- Unconditionally energy-stable for a perturbed energy

$$\widetilde{E}(\phi^{n+1}) = E(\phi^{n+1}) + k^2 \int_\Omega \frac{1}{4\varepsilon^2} |\delta_t \phi^{n+1}|^2 dx,$$

Theorem

- *Unconditionally unique solvable*
- *Convergence hypothesis (Idem* **MP***)*

$$\frac{k^{1/2}}{\varepsilon^4} < C \quad \text{and} \quad \lim_{(k,h)\to 0} \frac{k}{h^2} = 0.$$

Optimal Dissipation Scheme (OD2)

Aim: Design $f^k(\phi^{n+1},\phi^n)$, linear, second order accurate and

$$ND_{phobic}(\phi^{n+1},\phi^n) = O(k^2)$$

Idea: Using a Hermite quadrature formula,

$$\frac{F(\phi^{n+1}) - F(\phi^n)}{\phi^{n+1} - \phi^n} = \frac{1}{\phi^{n+1} - \phi^n} \int_{\phi^n}^{\phi^{n+1}} f(\phi) d\phi$$

$$= f(\phi^n) + \frac{f'(\phi^n)}{2}(\phi^{n+1} - \phi^n) + C\, f''(\phi^{n+\zeta})\,(\phi^{n+1} - \phi^n)^2$$

We define

$$f^k(\phi^{n+1},\phi^n) := f(\phi^n) + \frac{1}{2}(\phi^{n+1} - \phi^n) f'(\phi^n)$$

Properties:

- Second order
- Linear scheme
- Conditionally solvable ($k < 8\varepsilon^4/\gamma$)

Remark: We can not control the sign of $ND_{phobic}(\phi^{n+1},\phi^n)$

Splitting the potential term $F(\phi) = F_c(\phi) + F_e(\phi)$ with $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave) **OD2** approximation of the convex term and **BDF2** the non-convex one,

$$f^k(\phi^{n+1}, \phi^n, \phi^{n-1})$$

$$= f_c(\phi^n) + \frac{1}{2}(\phi^{n+1} - \phi^n) f_c'(\phi^n) + \frac{1}{2}\left(3 f_e(\phi^n) - f_e(\phi^{n-1})\right).$$

Properties:

- Second order
- Linear scheme
- Unconditionally solvable

Remark: We can not control the sign of $ND_{phobic}(\phi^{n+1}, \phi^n)$

Lagrange Multiplier Schemes.

Aim: Obtain a unconditionally energy-stable linear scheme.
Idea: **[Badia et al.]** Introduce a *"Lagrange multiplier"* $q(x,t) \in \boldsymbol{R}$ s. t.

$$f(\phi) = q\phi \quad \text{where} \quad q = \frac{1}{\varepsilon^2}(\phi^2 - 1)$$

Taking its time derivative equation with the initial condition:

$$q = \frac{1}{\varepsilon^2}(\phi^2 - 1) \quad \Longleftrightarrow \quad \begin{cases} \varepsilon^2 q_t = 2\phi\phi_t, \\ \varepsilon^2 q(0) = \phi(0)^2 - 1 \end{cases}$$

Weak reformulation: Find (ϕ, w, q) such that

$$\begin{cases} \langle \phi_t, \overline{w} \rangle + \gamma(\nabla w, \nabla \overline{w}) = 0 & \forall \overline{w} \in H^1(\Omega) \\ (\nabla \phi, \nabla \overline{\phi}) + (q\phi, \overline{\phi}) - (w, \overline{\phi}) = 0 & \forall \overline{\phi} \in H^1(\Omega) \\ \dfrac{\varepsilon^2}{2}(q_t, \overline{q}) - (\phi\, \phi_t, \overline{q}) = 0 & \forall \overline{q} \in L^2(\Omega) \end{cases}$$

Lagrange Multiplier Scheme (LM2)

$$\begin{cases} (\delta_t \phi^{n+1}, \overline{w}) + \gamma(\nabla w^{n+\frac{1}{2}}, \nabla \overline{w}) = 0 \\ (\nabla(\phi^n + \phi^{n+1})/2, \nabla \overline{\phi}) + (\widetilde{\phi}^{n+\frac{1}{2}}(q^n + q^{n+1})/2, \overline{\phi}) - (w^{n+\frac{1}{2}}, \overline{\phi}) = 0 \\ \dfrac{\varepsilon^2}{2}(\delta_t q^{n+1}, \overline{q}) - (\widetilde{\phi}^{n+\frac{1}{2}} \delta_t \phi^{n+1}, \overline{q}) = 0 \end{cases}$$

where

$$\widetilde{\phi}^{n+\frac{1}{2}} = \frac{1}{2}(3\phi^n - \phi^{n-1})$$

.

Properties:

- Second order
- Linear scheme
- Unconditionally solvable
- Unconditionally energy-stable for the modified energy

$$\widetilde{E}^n(\phi^n, q^n) = \int_\Omega \left(\frac{1}{2}|\nabla \phi^n|^2 + \frac{\varepsilon^2}{4}|q^n|^2 \right) dx$$

Time step adaptivity.

We have developed a new adaptive-in-time algorithm by using a criterion related to the 'residual energy law'.

Generic Algorithm:

Given ϕ^n, ϕ^{n-1},dt^{n-1}, dt^n, **resmax** and **resmin**:

1. Compute ϕ^{n+1} and
$$RE^{n+1} := \frac{E(\phi^{n+1}) - E(\phi^n)}{dt^n} + \|\nabla w^{n+1/2}\|^2_{L^2}.$$
2. If $|RE^{n+1}| > $ **resmax**, take $dt^n = dt^n/\theta$ and go to 1). $(\theta > 1)$
3. If $|RE^{n+1}| < $ **resmin**, take $dt^{n+1} = \theta dt^n$.
4. Take $t^{n+1} = t^n + dt^n$ and go to next time step.

Numerical Simulations. Spinodal decomposition. Comparative: OD2, MP, US2 and OD2-BDF2

- $\mathcal{P}_1$-cont. FE for ϕ_h, w_h, $\Omega = [0,1]^2$, $h = 1/90$, $\gamma = 10^{-4}$, $\varepsilon = 10^{-2}$, **resmax** $= 10$ and **resmin** $= 1$.
- In Newton's method, a tolerance parameter $tol = 10^{-3}$. The time-step is reduced in the case that the method does not converge in 10 iterations.
- Random initial data (the same for all the schemes).

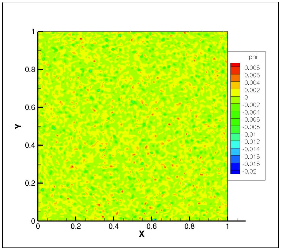

Figura: Random initial data

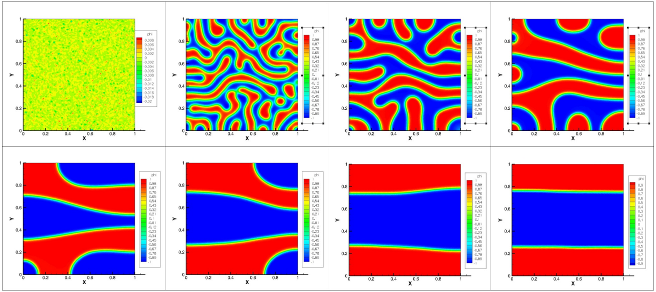

Figura: Dynamic of the model for the random initial condition

Mixing energy

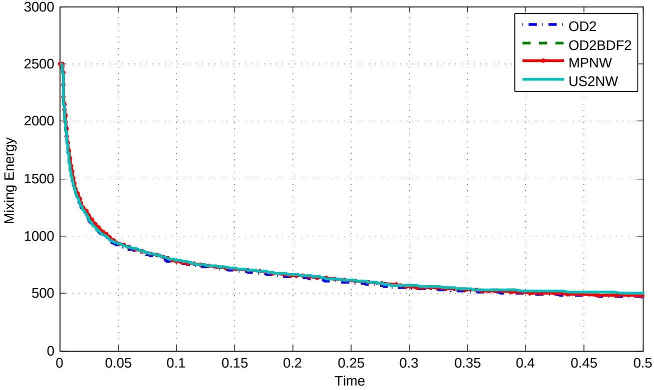

Figura: Mixing energy in [0, 0.5]

Mixing energy

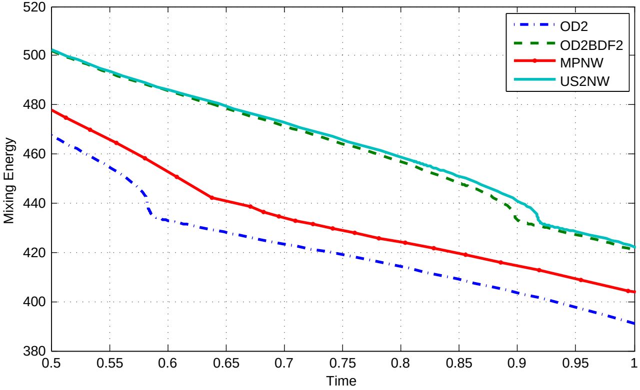

Figura: Mixing energy in [0.5, 1]

Mixing energy

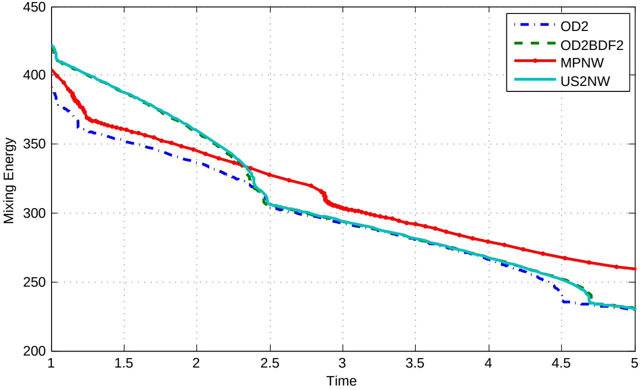

Figura: Mixing energy in [1, 5]

Mixing energy

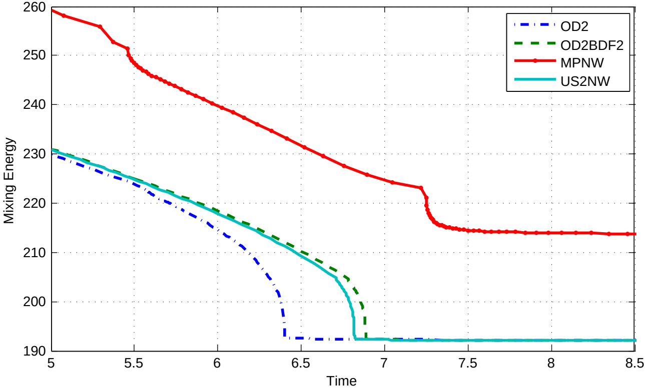

Figura: Mixing energy in [5, 8.5]

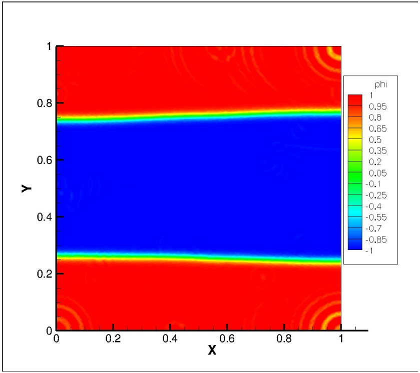

Figura: Equilibrium solution of MP

Time steps

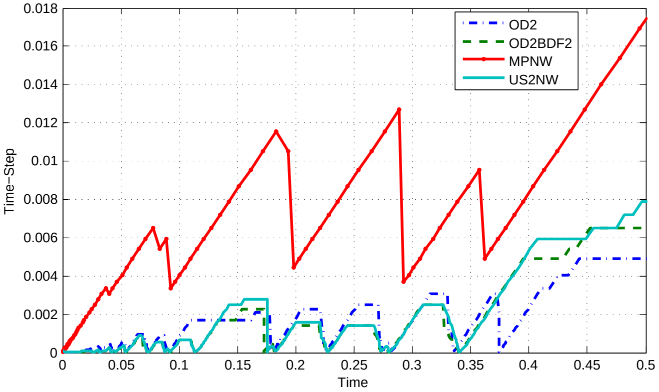

Figura: Time steps in [0, 0.5]

Time steps

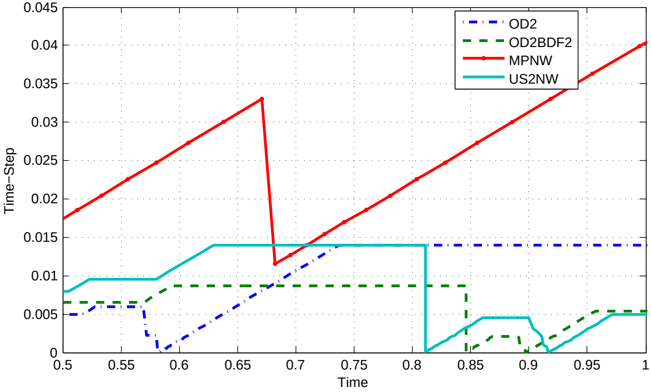

Figura: Time steps in [0.5, 1]

Time steps

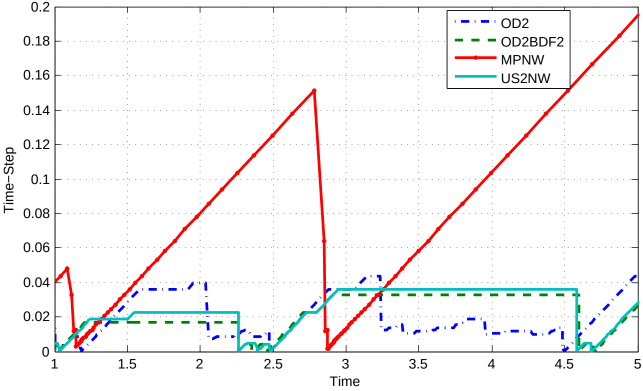

Figura: Time steps in [1, 5]

Time steps

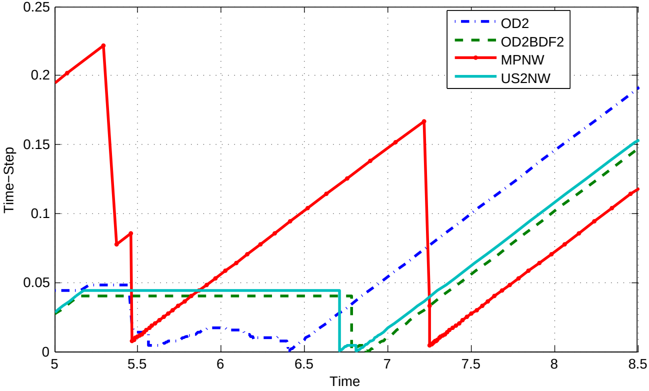

Figura: Time steps in [5, 8.5]

Time steps

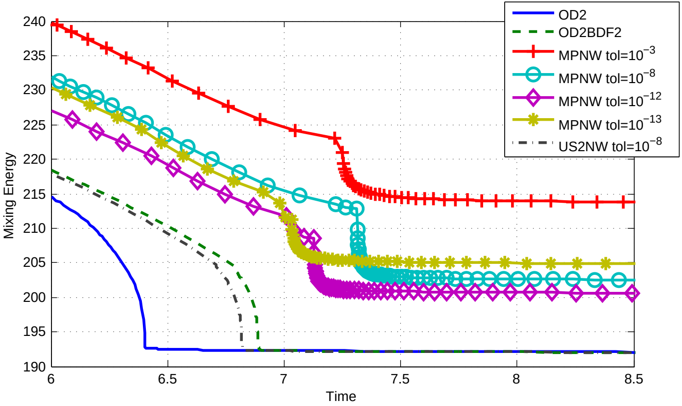

Figura: Mixing energy in [6, 8.5]

Numerical Simulations. Efficiency

Computational cost:

	MP	OD2	OD2-BDF2	US2
# Time steps	339	2642	4340	3691
# Linear systems solved	3896	3533	5687	12812

(**OD2** with constant time step $k = 10^{-4} \Rightarrow \simeq$ 80000 iterations)

Conclusions:

	MP	OD2	OD2-BDF2	US2	LM2
Linear	X	✓	✓	X	✓
Unconditionally Unique Solvable	X	X	✓	✓	✓
Conditionally Unique Solvable	✓	✓			
Unconditionally Energy-Stable $E(\phi)$	✓	X	X	X	X
Uncond. (Modified-Energy)-Stable $\widetilde{E}(\phi)$		X	X	✓	✓
One-Step Algorithm	✓	✓	X	X	X
Time-step Adaptivity	X	✓	✓	✓	X

- **OD2** time scheme.
- Finite element discretization in space, with ϕ_h and w_h in $\mathcal{P}_1$-cont. FE
- $\Omega = [0,1]^3$, $h = 1/30$, $\gamma = 10^{-4}$, $\varepsilon = 10^{-2}$, **resmax** $= 10$ and **resmin** $= 1$.
- Random initial data.

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THANK YOU FOR YOUR ATTENTION!