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Environmental Fluid Modelling

Fundamentals of Computational Fluid Dynamics

(1) Weak Formulation of Governing Equation

Governing Equation

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nabla (\mathbf{v} \nabla \mathbf{u})$$

Boundary Condition

$$u = u^* (on\Gamma_1)$$
 $v\nabla u = \tau^* (on\Gamma_2)$

Method of Weighted Residuals

$$\int_{\Omega} w \frac{\partial u}{\partial t} d\Omega + \int_{\Omega} w u \cdot \nabla u d\Omega = \int_{\Omega} w \nabla (v \nabla u) d\Omega$$

Solve the weak form of the governing equation

- · by dividing the target region into a set of cells (elements)
- by assembling the cell-wisely integrated equation into a whole matrix form

There are multiple methods with respect to the weighting functions

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(a) Finite Difference Method

- · satisfy the governing equation on points
- no conservation of convection term
- · applicable to arbitrary shape of region by body-fitted grid

$$w=1$$
 (on r_{α}) $w=0$ (others)

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = v \nabla^2 u \qquad (\text{on } r_{\alpha})$$

(b) Finite Volume Method

- · satisfy the governing equation averagely in each cell
- · conservation of convection term for high Reynolds number flow
- applicable to arbitrary shape of region by body-fitted grid or unstructured grids

w=1 (in Ω_{α}) w=0 (others)

$$\frac{\partial u}{\partial t} + \frac{1}{\Omega_{\alpha}} \int_{\Gamma_{\alpha}} u(u \cdot n) d\Gamma = \frac{1}{\Omega_{\alpha}} \int_{\Gamma_{\alpha}} v(\nabla u \cdot n) d\Gamma$$

(c) Finite Element Method (Galerkin Method)

- · satisfy the governing equation approximately in the region
- no conservation of convection term
- applicable to arbitrary shape of region by body-fitted grid or unstructured mesh

 $w \!=\! N \quad \mathrm{where} \ u \!=\! \overline{u} \cdot N$

$$\left(\int_{\Omega_{\alpha}} NNd\Omega\right) \frac{\partial \overline{u}}{\partial t} + \left(\int_{\Omega_{\alpha}} N(u \cdot \nabla)Nd\Omega\right) \overline{u} = v \left(\int_{\Omega_{\alpha}} \nabla N \nabla Nd\Omega\right) \overline{u} - \int_{\Gamma_{\alpha}} N(v \nabla u) d\Omega$$

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(2) Algorism to Solve Incompressible NS Equation

(a) MAC Method (Marker and Cell) of Harlow and Welch (1965)

•	FDM, FVM, FEM
•	Unsteady (and steady)
	Staggered Grid

 $\frac{\mathbf{u}^{n+1} - \mathbf{u}}{\Delta t} = -\nabla \cdot (\mathbf{u}\mathbf{u}) + \frac{1}{Rc} \nabla^2 \mathbf{u} - \nabla p^{n+1}$ (1) $\nabla^2 p^{n+1} = \frac{\nabla \cdot \mathbf{u}}{\Delta t} - \nabla \cdot \mathbf{F}$ (2)

Solve this by SOR (Successive Over Relaxation). Boundary condition for p on the body surface is given by $\nabla p = \frac{\nabla^2 u}{R_0}$.

(b) SMAC Method (Simplified MAC) of Amsden and Harlow (1970)

$$\frac{\mathbf{u}^* - \mathbf{u}}{\Delta t} = -\nabla \bullet (\mathbf{u}\mathbf{u}) + \frac{1}{R_r} \nabla^2 \mathbf{u} - \nabla \mathbf{p}$$
(3)

Introduce irrotational velocity (potential flow)

$$\begin{aligned} \mathbf{u}^{n+1} &= \mathbf{u}^* + \mathbf{u}^C \\ \mathbf{u}^C &= \nabla \Phi \\ \nabla^2 \Phi &= -\nabla \bullet \mathbf{u}^* \quad \left(: \nabla \bullet \mathbf{u}^{n+1} = 0\right) \end{aligned}$$
 (4)

where

$$\delta p = p^{n+1} - p = -\frac{\Phi}{\Delta t}$$
(5)
$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^*}{\Delta t} = -\nabla \delta p$$
(6)

Boundary condition for Φ on the body surface is given by $\nabla \Phi = 0$.

(c) Projection method of Chorin (1968) - Velocity-Pressure Simultaneous Iteration

No direct boundary condition for pressure. Consider a pseudo time-developing equation for $~\delta p\,.$

$$\frac{\delta p^{m+1} - \delta p^{m}}{\omega} = \frac{\nabla \bullet \mathbf{u}^{*}}{\Delta t} - \nabla^{2} \delta p^{m}$$
$$= \nabla \bullet \left(\frac{\mathbf{u}^{*}}{\Delta t} - \nabla \delta p^{m} \right)$$
$$= \frac{\nabla \bullet \mathbf{u}^{m}}{\Delta t}$$
(7)

where ω is pseudo time-step and, at the same time, relaxation factor in iterative relaxation method. The upper limit of ω is given by considering the diffusion number for stability. m is the number of iteration and the convergence is achieved when $\delta p^{m+1} - \delta p^m < \epsilon$. The resultant u^m satisfies the continuity equation and, therefore, $u^{n+1} = u^{m1}$. No need of the boundary condition for pressure.

(d) HSMAC Method (Highly Simplified MAC) by Hirt and Cook (1972)

Solve Eq. (2) in the following simply approximated way to reduce the computational time.

$$\frac{\partial^2 \mathbf{p}}{\partial x^2} = \frac{\mathbf{p}_{i-1} - 2\mathbf{p}_i + \mathbf{p}_{i+1}}{\Delta x^2} \approx -\frac{2\mathbf{p}_i}{\Delta x^2} \tag{8}$$

$$p^{m+1} = -\frac{\omega \nabla \bullet \mathbf{u}^m}{2\Delta t (\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta x^2})}$$
(9)

If resultant \mathbf{u}^m satisfies the continuity equation, it is \mathbf{u}^{n+1} . In fact, the pressure silver in HSMAC is regarded as the Newton iteration: $p^{m+1} = p^m - \frac{(\nabla \bullet \mathbf{u}^m)}{d(\mathbf{v}^{-m})}$

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$$d_{\text{dp}} = \frac{d(\nabla \cdot \mathbf{u}^m)}{dp}$$

(e) SIMPLE Method (Semi-Implicit Method for Pressure-Linked Equation) of Patankar and Spalding (1980)

- FVM
- Steady and unsteady
- Staggered Grid

Discretised NS Equation is

$a_{i+\frac{1}{2}}u^{*}_{i+\frac{1}{2}} = \sum_{nb}a_{nb}u^{*}_{nb} + A_{i+\frac{1}{2}}(p_{i+1} - p_{i})$	(10)
$a_{j+\frac{1}{2}}v^{*}_{j+\frac{1}{2}} = \sum_{nb} a_{nb}v^{*}_{nb} + A_{j+\frac{1}{2}}(p_{j+1} - p_{j})$	(11)

Solve these equation implicitly by using initial guess of p. But the coefficients a are not updated, so that this is called "semi-implicit". The resultant u^* and v^* do not satisfy the continuity equation. Therefore, the descritised Poisson equation for δp is solved.

$a_{i,j}\delta p_{i,j} = \sum_{nb} a_{nb} \delta p_{nb} + b$	(12)			
Then the velocities are corrected.				
$u_{i+\frac{1}{2}}=u^{*}_{i+\frac{1}{2}}+d_{i+\frac{1}{2}}(\delta p_{i+1}-\delta p_{i})$	(13)			
$v_{j+\frac{1}{2}} = v^*{}_{j+\frac{1}{2}} + d_{j+\frac{1}{2}} (\delta p_{j+1} - \delta p_{j})$	(14)			

Application to unsteady flows is also available.

(f) Pseudo-Compressibility Method of Chorin (1967)

- FDM, FVM, FEM
- Steady (and unsteady)
- Collocation grid (cell-centred)

The difficulty to solve the equation system for incompressible flow stems from the difference of type between equations for velocity and pressure (parabolic and elliptic). On the other hand, those for compressible flow are both time-developing. By analogy from compressible flow, pseudo-compressibility is introduced in the solver of incompressible flow. The resultant velocity satisfies the continuity equation (incompressibility), but the velocity on the way to reach the steady state does not have any sense.

$$\frac{\partial \mathbf{u}}{\partial \tau} = -\nabla \bullet (\mathbf{u}\mathbf{u}) + \frac{1}{Re} \nabla^2 \mathbf{u} - \nabla \mathbf{p}$$
(15)

$$\frac{\partial \mathbf{p}}{\partial \tau} = -c^2 \nabla \cdot \mathbf{u}$$
 (16)

Mainly, implicit time integration is used, so that fast solvers of inverse matrix like the Newton method is necessary. Application to unsteady flow is also studied.

(3) Variable Decomposition and Checker Board (Why Staggered?)

When updating velocity by the gradient of the pressure, sometimes we suffer artificial oscillation of either of velocity (called "wiggle") and pressure (called "checkerboard"). Consider 1D space.

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$$\frac{\hat{o}p}{\hat{o}x} = \frac{\frac{p_{i-1} + p_i}{2} - \frac{p_i + p_{i+1}}{2}}{\Delta x} = \frac{p_{i-1} - p_{i+1}}{2\Delta x}$$
(17)

There is no use of p_i and, therefore, cell-wise oscillation of pressure occurs without oscillating velocity. If $\nabla \cdot \mathbf{u}$ is satisfied, there is no suppression on the pressure oscillation. In 2D, oscillated pressure contour looks a checkerboard.

To avoid this type of oscillation, velocities should be defined on the edge of the control volume for pressure (which guarantees the incompressibility). This is called "staggered grids". In case of the pseudo-compressibility method, velocities and pressure are defined at the same point, such as cell-centre.

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(4) Grid Systems

(a) Body-Fitted (Boundary-Fitted) Grids

In general, the region of interest has arbitrary shape, so that the grid system becomes curvilinear fitting to the bodies and boundaries. By the chain rule, the difference along the curvilinear $\,\xi_i\,$ has the form of

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$$\frac{\partial \Phi}{\partial x_{k}} = \sum_{i} \frac{\partial \xi_{i}}{\partial x_{k}} \frac{\partial \Phi}{\partial \xi_{i}}$$
(18)

In the FVM formulation,

$$\begin{split} & \frac{\partial \Phi}{\partial x_k} = \frac{1}{V} \int \frac{\partial \Phi}{\partial x_k} \, dV = \frac{1}{V} \oint \Phi dS_k \\ & = \frac{1}{V} \left((\Phi S_k^i)_{j+\frac{1}{2}} - (\Phi S_k^i)_{j+\frac{1}{2}} + (\Phi S_k^j)_{j+\frac{1}{2}} - (\Phi S_k^j)_{j-\frac{1}{2}} \right) \end{split}$$
(19)

where S_k^i is k Cartesian component of the area vector along the i direction. Therefore, $\frac{S_k^i}{V}$ is the same as $\frac{\partial \xi_i}{\partial x_k}$ in Eq. (18).

(b) Unstructured Grids

If grids are not in order, in other words, normalised grids in the reference space are not topologically expressed by the combination of cubic blocks, they are called unstructured grids (mesh).

$$\frac{\partial \Phi}{\partial x_{k}} = \frac{1}{V} \int \frac{\partial \Phi}{\partial x_{k}} dV = \frac{1}{V} \oint \Phi dS_{k} = \frac{1}{V} \sum_{\alpha} \Phi S_{k}^{\alpha}$$
(20)

where subscripts α indicates each face shared with the neighbouring cell. S_k^{α}

is $\,k\,$ Cartesian component of the area vector of the face $\,\alpha\,.$

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(5) Accuracy of Differencing Scheme

(a) Space Derivative

2nd-order Central Differencing

Taylor expansion

 $\mathbf{u}_{i\pm 1} \approx \mathbf{u}_i \pm \Delta \frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\Delta^2}{2'} \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} \pm \frac{\Delta^3}{3'} \frac{\partial^3 \mathbf{u}}{\partial \mathbf{x}^3} + \frac{\Delta^4}{4'} \frac{\partial^4 \mathbf{u}}{\partial \mathbf{x}^4} \cdots$

$$\frac{\delta u}{\delta x} \approx \frac{u_{i+1} - u_{i-1}}{2\Delta} = \frac{\partial u}{\partial x} + \frac{\Delta^2}{6} \frac{\partial^3 u}{\partial x^3} + \dots = \frac{\partial u}{\partial x} + O(\Delta^2)$$
 2nd-order accuracy

Second Derivative

$$\frac{\delta^2 \mathbf{u}}{\delta \mathbf{x}^2} \approx \frac{\frac{\mathbf{u}_{i+1} - \mathbf{u}_i}{\Delta} - \frac{\mathbf{u}_i - \mathbf{u}_{i-1}}{\Delta}}{\Delta} = \frac{\mathbf{u}_{i+1} - 2\mathbf{u}_i + \mathbf{u}_{i-1}}{\Delta^2} = \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + \frac{\Delta^2}{12} \frac{\partial^4 \mathbf{u}}{\partial \mathbf{x}^4} + \dots = \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + O\left(\Delta^2\right)$$
2nd-order accuracy

u_{i-1}

 $\frac{\partial u}{\partial x_{i}}$

 \mathbf{u}_{i^+}

4th-order Central Differencing

$$\begin{array}{c|c} & & & & & \\ \hline & & & & \\ u_{i\cdot 2} & & u_{i\cdot 1} & & \\ \hline & & & & \\ \frac{\partial u_i}{\partial x_i} & & & u_{i+2} \end{array}$$

Taylor expansion

$$u_{i\pm 2} \approx u_i \pm 2\Delta \frac{\partial u}{\partial x} + \frac{(2\Delta)^2}{2!} \frac{\partial^2 u}{\partial x^2} \pm \frac{(2\Delta)^3}{3!} \frac{\partial^3 u}{\partial x^3} + \frac{(2\Delta)^4}{4!} \frac{\partial^4 u}{\partial x^4} \cdots$$

First Derivative

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Ist-order Upwind Differencing

$$\begin{array}{c} & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & &$$

2nd-order Upwind Differencing



3rd-order Upwind Differencing



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(b) Time Derivative

Governing Equation
$$\frac{\partial u}{\partial t} = f(u), \quad u = u_0 \text{ at } t = 0$$

time developing: initial-value problem
1st-order Explicit Euler Scheme
 $u^n \qquad u^{n+1}$

uⁿ⁺¹

1st-order accuracy

Taylor expansion

$$\begin{split} u^{n+1} &= u^n + \Delta t \frac{\partial u}{\partial t} + \frac{\Delta t^2}{2!} \frac{\partial^2 u}{\partial t^2} + \frac{\partial^3 u}{\partial t^3} + \frac{\Delta t^4}{4!} \frac{\partial^4 u}{\partial t^4} \cdots \\ &= u^n + \Delta t \frac{\partial u}{\partial t} \Big|^n + O(\Delta t^2) \\ &= u^n + \Delta t \cdot f(u^n) + O(\Delta t^2) \end{split}$$

$$\frac{\delta u}{\delta t} \approx \frac{u^{n+1} - u^n}{\Delta t} = \frac{\partial u}{\partial t} + \frac{\Delta t}{2} \frac{\partial^2 u}{\partial t^2} + \dots = \frac{\partial u}{\partial t} + O(\Delta t)$$

2nd-order Explicit Adams-Bashforth Scheme

m-th-order Explicit Runge-Kutta Scheme



m-th-order accuracy

1st-order Implicit Euler Differencing

 $u^{n+1} = u^n + \Delta t \cdot f(u^{n+1}) + O(\Delta t^2)$

1st-order accuracy

2nd-order Implicit Trapezoidal Scheme(Crank-Nicolson Scheme for Diffusion Term)

$$\begin{split} u^{n+1} &= u^n + \Delta t \frac{\partial u}{\partial t} \Big|^n + \frac{\Delta t^2}{2t} \left(\frac{\frac{\partial u}{\partial t} \Big|^{n+1} - \frac{\partial u}{\partial t} \Big|^n}{\Delta t} + O(\Delta t) \right) + O(\Delta t^3) \\ &= u^n + \Delta t \frac{\partial u}{\partial t} \Big|^n + \frac{\Delta t}{2} \left(\frac{\partial u}{\partial t} \Big|^{n+1} - \frac{\partial u}{\partial t} \Big|^n \right) + O(\Delta t^3) \\ &= u^n + \frac{\Delta t}{2} \frac{\partial u}{\partial t} \Big|^{n+1} + \frac{\Delta t}{2} \frac{\partial u}{\partial t} \Big|^n + O(\Delta t^3) \\ &= u^n + \Delta t \frac{f(u^{n+1}) + f(u^n)}{2} + O(\Delta t^3) \end{split}$$

2nd-order accuracy

(c) Effect of Numerical Error

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Ex.1 Convection Term : 1st-order Upwind Differencing Diffusion Term : 2nd-order Central Differencing

$$\begin{split} & \frac{\delta u}{\delta x}\approx \frac{u_1-u_{1-1}}{\Delta}=\frac{\partial u}{\partial x}-\frac{\Delta}{2}\frac{\partial^2 u}{\partial x^2}+\cdots=\frac{\partial u}{\partial x}+O(\Delta)\\ & \frac{\delta^2 u}{\delta x^2}\approx \frac{u_{1+1}-u_1}{\Delta}-\frac{u_1-u_{1-1}}{\Delta}=\frac{u_{1+1}-2u_1+u_{1-1}}{\Delta^2}=\frac{\partial^2 u}{\partial x^2}+\frac{\Delta^2}{12}\frac{\partial^4 u}{\partial x^4}+\cdots=\frac{\partial^2 u}{\partial x^2}+O(\Delta^2) \end{split}$$

1D Transport Equation (U > 0)

$$\begin{split} &\frac{\partial u}{\partial t} = -U \frac{\partial u}{\partial x} + v \frac{\delta^2 u}{\delta x^2} \\ &= -U \left[\frac{\partial u}{\partial x} - \frac{\Delta}{2 \partial x^2} + \frac{\Delta^2}{6} \frac{\partial^3 u}{\partial x^3} - \frac{\Delta^3}{24} \frac{\partial^4 u}{\partial x^4} + O\left(\Delta^4\right) \right] + v \left(\frac{\partial^2 u}{\partial x^2} + \frac{\Delta^2}{12} \frac{\partial^4 u}{\partial x^4} + O\left(\Delta^3\right) \right) \\ &= -U \frac{\partial u}{\partial x} + \frac{\left(v + \frac{U\Delta}{2}\right)}{\partial x^2} \frac{\partial^2 u}{\partial x^2} - \frac{U\Delta^2}{6} \frac{\partial^3 u}{\partial x^3} + \left(\frac{U\Delta^3}{24} + \frac{v\Delta^2}{12} \right) \frac{\partial^4 u}{\partial x^4} + O\left(\Delta^3\right) \end{split}$$

artificial diffusion

Ex.2 Convection Term : 3rd-order Upwind Differencing Diffusion Term : 2nd-order Central Differencing

$$\begin{split} & \frac{\delta u}{\delta x} \approx \frac{2u_{i+1} + 3u_i - 6u_{i-1} + u_{i-2}}{6\Delta} = \frac{\partial u}{\partial x} + \frac{\lambda^2}{2} \frac{\partial^4 u}{\partial x^4} + \cdots = \frac{\partial u}{\partial x} + O\left(\lambda^3\right) \\ & \frac{\delta^2 u}{\delta x^2} \approx \frac{u_{i+1} - u_i}{\Delta} - \frac{u_i - u_{i-1}}{\Delta} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\lambda^2}{12} \frac{\partial^4 u}{\partial x^4} + \cdots = \frac{\partial^2 u}{\partial x^2} + O\left(\lambda^2\right) \end{split}$$

1D Transport Equation (U > 0)

$$\begin{split} &\frac{\partial \mathbf{u}}{\partial t} = -\mathbf{U}\frac{\delta \mathbf{u}}{\delta \mathbf{x}} + \mathbf{v}\frac{\delta^2 \mathbf{u}}{\delta \mathbf{x}^2} \\ &= -\mathbf{U}\left(\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\mathbf{A}^3}{2}\frac{\partial^4 \mathbf{u}}{\partial \mathbf{x}^4} + \mathbf{O}\left(\mathbf{A}^4\right)\right) + \mathbf{v}\left(\frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + \frac{\mathbf{A}^2}{12}\frac{\partial^4 \mathbf{u}}{\partial \mathbf{x}^4} + \mathbf{O}\left(\mathbf{A}^3\right)\right) \\ &= -\mathbf{U}\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{v}\frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + \underbrace{\left(-\frac{\mathbf{U}\mathbf{A}^3}{2} + \frac{\mathbf{v}\mathbf{A}^2}{12}\right)\frac{\partial^4 \mathbf{u}}{\partial \mathbf{x}^4} + \mathbf{O}\left(\mathbf{A}^3\right) \\ & \text{artificial dissipation} \end{split}$$

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Ex.3 Time-Derivative Term: 1st-order Euler Scheme

$$\begin{split} &\frac{\delta u}{\delta t} \approx \frac{u^{n+1} - u^n}{\Delta t} = \frac{\delta u}{\delta t} + \frac{\Delta t}{2} \frac{\partial^2 u}{\partial t^2} + O\left(\Delta t^2\right) \\ &\approx \frac{\delta u}{\partial t} + \frac{\Delta t}{2} \frac{\partial}{\partial t} \left(\frac{\Delta u}{\partial t}\right) \\ &= \frac{\delta u}{\partial t} + \frac{\Delta t}{2} \frac{\partial}{\partial t} \left(-U \frac{\partial u}{\partial x} + V \frac{\partial^2 u}{\partial x^2}\right) \\ &= \frac{\delta u}{\partial t} - \frac{U \Delta t}{2} \frac{\partial^2 u}{\partial t^2} + \frac{V \Delta t}{2} \frac{\partial^2 u}{\partial t^2} \\ &= \frac{\delta u}{\partial t} - \frac{U \Delta t}{2} \frac{\partial^2 u}{\partial t} \left(\frac{\partial u}{\partial t}\right) + \frac{V \Delta t}{2} \frac{\partial^2}{\partial x^2} \left(\frac{\partial u}{\partial t}\right) \\ &= \frac{\delta u}{\partial t} - \frac{U \Delta t}{2} \frac{\partial}{\partial t} \left(-U \frac{\partial u}{\partial x} + V \frac{\partial^2 u}{\partial x^2}\right) + \frac{V \Delta t}{2} \frac{\partial^2}{\partial x^2} \left(-U \frac{\partial u}{\partial x} + V \frac{\partial^2 u}{\partial x^2}\right) \\ &= \frac{\delta u}{\partial t} + \frac{U^2 \Delta t}{2} \frac{\partial^2 u}{\partial x^2} - U v \Delta t \frac{\partial^2 u}{\partial x^3} + \frac{v^2 \Delta t}{\partial x} \frac{\partial^4 u}{\partial x^4} \\ & \text{artificial diffusion} \end{split}$$

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