Everybody's Recipe for Making Good Diffusion Schemes

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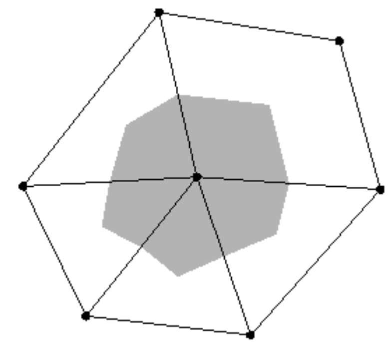
Common Approach

Integral form for diffusion:

$$\int_\Omega u_t \;=\; \int_\Omega \nabla^2 u = \oint_{\partial\Omega} \nabla u \cdot \mathbf{n}\, dA$$



Compute the interface gradient.

Bad diffusion schemes lack high-frequency damping:

Large errors, poor convergence, lose consistency…….

Good diffusion schemes have a *damping* term:

Finite-Volume: edge-term.

High-Order Schemes: penalty term.

Residual-Distribution: ?

Do we really know how to make a diffusion scheme?

Hyperbolic Model for Diffusion

Diffusion Equation (Parabolic)

$$u_t = \nu \, u_{xx}$$

Hyperbolic Model for Diffusion

$$\begin{aligned} u_t &= \nu \, p_x \\ p_t &= (u_x - p)/T_r \end{aligned}$$

$$\lambda = \pm\sqrt{\frac{\nu}{T_r}}$$

Discretization

difficult

Discretization

easy

?

Diffusion Scheme

Advection Scheme

From Advection to Diffusion

Diffusion Equation (Parabolic)

$$u_t = \nu\, u_{xx}$$

Hyperbolic Model for Diffusion

$$\begin{aligned} u_t &= \nu\, p_x \\ p_t &= (u_x - p)/T_r \end{aligned}$$

Two models are equivalent if $p = u_x$.

Derive a diffusion scheme from an advection scheme.

1. Discretize the hyperbolic system by an **advection** scheme:

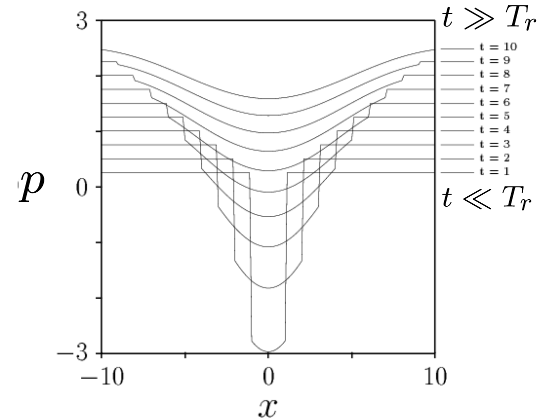
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -Res_{j,1}^n, \qquad \frac{p_j^{n+1} - p_j^n}{\Delta t} = -Res_{j,2}^n - \frac{1}{T_r} p_j^n.$$

2. Replace the second equation by a direct approximation of $p = u_x$:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -Res_{j,1}^n, \qquad p_j^n = \text{least-squares gradient, for example}$$

The result is a time-accurate **diffusion** scheme. (no need to store extra variables)

Relaxation Time



The CFL condition:

$$\Delta t \leq \frac{\Delta x}{\sqrt{\nu / T_r}}$$

Keep the hyperbolic behavior over every time step:

$$\Delta t_{\mathsf{max}} \equiv \frac{\Delta x}{\sqrt{\nu / T_r}} = \alpha T_r$$

Solve for Tr:

$$T_r = \frac{\Delta x^2}{\alpha^2 \nu}$$

The CFL condition becomes

$$\Delta t \leq \frac{1}{\alpha} \frac{\Delta x^2}{\nu}$$

General Form:

$$T_r = \frac{L_r^2}{\alpha^2 \nu}, \quad L_r = \frac{\Delta x}{D}$$

$$D = \begin{cases} 1 & \text{in 1D} \\ 2 & \text{in 2D} \\ 3 & \text{in 3D} \end{cases}$$

Recipe for Making Good Diffusion Schemes

$$u_t = \nu u_{xx}$$

1. Discretize the hyperbolic system by an advection scheme.

$$\mathbf{U}_t + \mathbf{F}_x = \mathbf{Q}$$

$$\mathbf{U} = \begin{bmatrix} u \\ p \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} -\nu p \\ -u/T_r \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} 0 \\ -p/T_r \end{bmatrix}.$$

2. Ignore the discrete equation for p, and approximate $p = u_x$ directly.

3. The result is a time-accurate diffusion scheme, a good one!

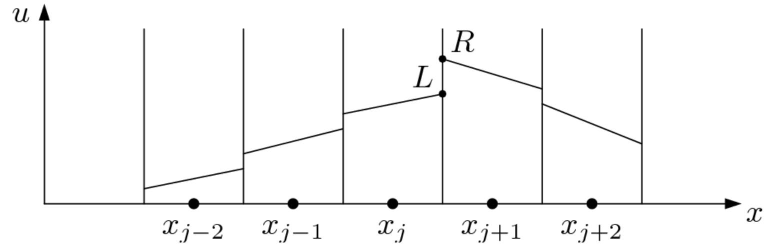
Derived diffusion scheme:

1. Automatically equipped with a damping term (edge/penalty term)
2. Implemented in the same way as a corresponding advection scheme.

This recipe is applicable to various discretization methods.

1D Finite-Volume Scheme

1. Discretize the hyperbolic system:



Finite-Volume Method:

$$\frac{d\mathbf{U}_j}{dt} = -\frac{1}{\Delta x}\left[\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}\right] + \frac{1}{\Delta x}\int_{I_j} \mathbf{Q}\, dx$$

Upwind Flux:

$$\mathbf{F}_{j+1/2} = \frac{1}{2}\left[\mathbf{F}_R + \mathbf{F}_L\right] - \frac{\nu\alpha}{2\Delta x}(\mathbf{U}_R - \mathbf{U}_L)$$

$$\mathbf{U} = \begin{bmatrix} u \\ p \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} -\nu p \\ -u/T_r \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} 0 \\ -p/T_r \end{bmatrix}.$$

2. Discard the second component to get a diffusion scheme:

$$\frac{du_j}{dt} = -\frac{1}{\Delta x}\left[f_{j+1/2} - f_{j-1/2}\right]$$

$$f_{j+1/2} = -\frac{\nu}{2}\left[p_R + p_L\right] - \frac{\nu\alpha}{2\Delta x}(u_R - u_L)$$

Consistent part **Damping**

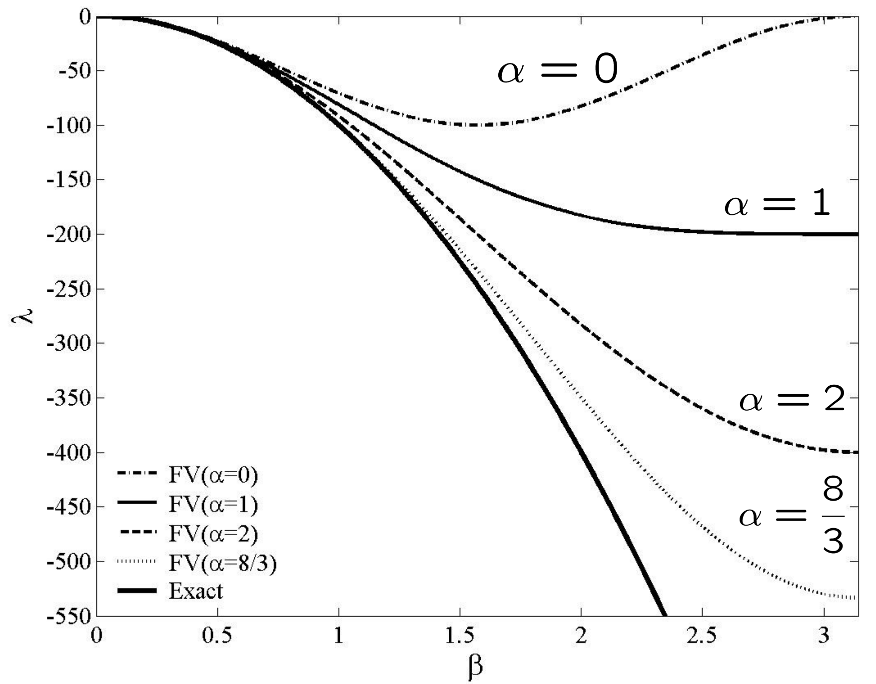
The damping term comes from the dissipation of the advection scheme.

Effect of Damping Term

Fourier transformed: $u_0 \exp(i\beta x/\Delta x)$

$$\frac{du_0}{dt} = -\frac{\nu}{\Delta x^2}\left(\sin^2\beta + 2\alpha\sin^4\frac{\beta}{2}\right)u_0$$

Consistent part **Damping**



Truncation Error:

$$\frac{du_j}{dt} = \nu u_{xx} + \nu u_{xxxx}\left(\frac{1}{3} - \frac{\alpha}{8}\right)\Delta x^2 + O(\Delta x^4)$$

The parameter α controls damping: 4th-order accurate for $\alpha = 8/3$.

Two Dimensions

$$u_t = \nu (u_{xx} + u_{yy})$$

Hyperbolic Model:

$$\mathbf{U}_t + \mathbf{F}_x + \mathbf{G}_y = \mathbf{Q}$$

$$\mathbf{U} = \begin{bmatrix} u \\ p \\ q \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} -\nu p \\ -u/T_r \\ 0 \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} -\nu q \\ 0 \\ -u/T_r \end{bmatrix}, \quad \mathbf{Q} = \begin{bmatrix} 0 \\ -p/T_r \\ -q/T_r \end{bmatrix}.$$

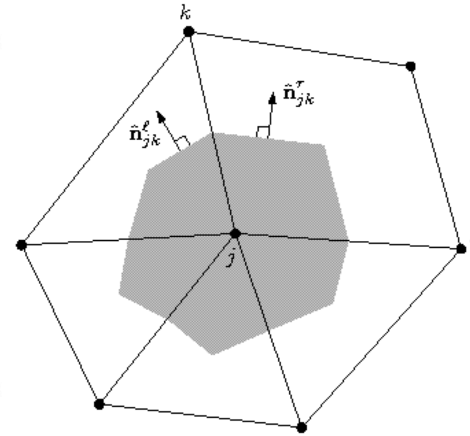
Equivalent to the diffusion equation when $p = u_x, q = u_y$

Absolute Jacobian:

$$|\mathbf{A}_n| = \mathbf{R}_n \mathbf{\Lambda}_n \mathbf{R}_n^{-1} = \sqrt{\frac{\nu}{T_r}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & n_x^2 & n_x n_y \\ 0 & n_x n_y & n_y^2 \end{bmatrix}.$$

The first component is all we need.

Node-Centered FV Schemes



1. Discretize hyperbolic system: Edge-based advection scheme:

$$\frac{d\mathbf{U}_j}{dt} = -\frac{1}{V_j}\sum_{k\in\{K_j\}} \Phi_{jk}A_{jk} + \frac{1}{V_j}\int_{\Omega_j} \mathbf{Q}\, dxdy$$

$$\Phi_{jk} = \frac{1}{2}\left[\mathbf{H}_{jk}(\mathbf{U}_R) + \mathbf{H}_{jk}(\mathbf{U}_L)\right] - \frac{1}{2}\left|\mathbf{A}_n\right|(\mathbf{U}_R - \mathbf{U}_L)$$

2. Discard the second and third components to get a diffusion scheme:

$$\frac{du_j}{dt} = -\frac{1}{V_j}\sum_{k\in\{K_j\}} \phi_{jk}A_{jk}$$

Diffusive flux:

$$\begin{aligned}\phi_{jk} &= -\frac{\nu}{2}\left[(p,q)_R + (p,q)_L\right]\cdot\hat{\mathbf{n}}_{jk} - \frac{\nu\alpha}{2L_r}(u_R - u_L) \\ &= -\frac{\nu}{2}\left[(\nabla u)_j + (\nabla u)_k\right]\cdot\hat{\mathbf{n}}_{jk} - \frac{\nu\alpha}{2L_r}(u_R - u_L)\end{aligned}$$

Consistent part **Damping**

Widely-used Avg-LSQ scheme can be reproduced by special choice of alpha.

The Green-Gauss scheme corresponds to using the Green-Gauss gradient for (p,q).

Length Scale and Skewness

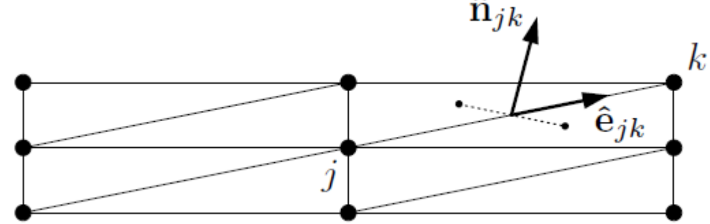
Derived diffusion scheme:

$$\phi_{jk} = -\frac{\nu}{2}\left[(\nabla u)_j + (\nabla u)_k\right] \cdot \hat{\mathbf{n}}_{jk} - \frac{\nu\alpha}{2L_r}(u_R - u_L)$$

Length scale is defined as

$$L_r = \frac{1}{2}|\Delta \mathbf{l}_{jk} \cdot \hat{\mathbf{n}}_{jk}| = \frac{1}{2}\Delta l_{jk}|\hat{\mathbf{e}}_{jk} \cdot \hat{\mathbf{n}}_{jk}|$$

Skewness measure



Damping is amplified for highly-skewed grids.

Widely-used Avg-LSQ scheme:

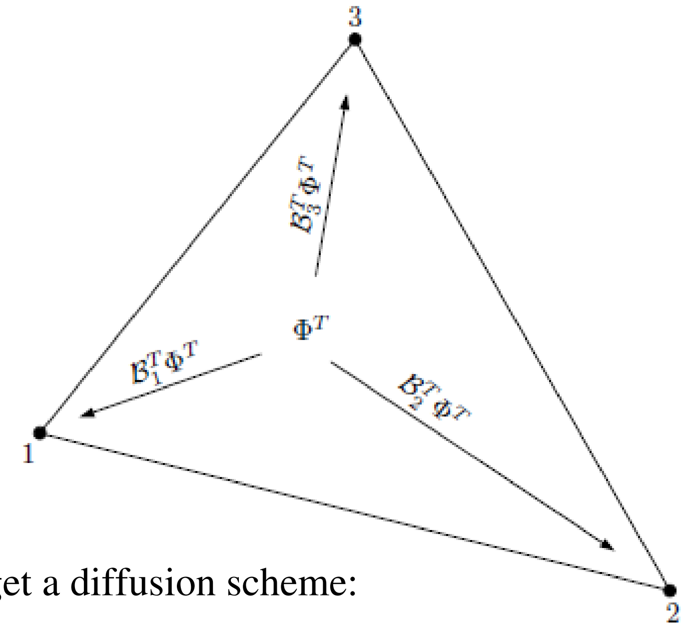
$$\phi_{jk} = -\frac{\nu}{2}\left[(\nabla u)_j + (\nabla u)_k\right] \cdot \hat{\mathbf{n}}_{jk} - \left(\hat{\mathbf{e}}_{jk} \cdot \hat{\mathbf{n}}_{jk}\right)(u_R - u_L)$$

It loses damping for highly-skewed grids.

The derived diffusion scheme is very accurate and robust for highly-skewed grids.

Residual-Distribution Schemes

- **Lax-Wendroff Scheme:**



1. Discretize the hyperbolic system:

$$\frac{d\mathbf{U}_j}{dt} = \frac{1}{V_j}\sum_{T\in\{T_j\}} \mathcal{B}_j^T \Phi^T,$$

$$\Phi^T = \int_T (-\mathbf{A}\mathbf{U}_x - \mathbf{B}\mathbf{U}_y + \mathbf{Q})\, dxdy$$

$$\mathcal{B}_i^T = \frac{1}{3}\mathbf{I} + \frac{h}{\sqrt{\nu/T_r}}(\mathbf{A},\mathbf{B})\cdot\mathbf{n}_i$$

2. Discard the second and third components to get a diffusion scheme:

$$\frac{du_j}{dt} = \frac{1}{V_j}\sum_{T\in\{T_j\}}\left[\frac{1}{3}\phi^T - \frac{\nu\alpha}{2}\left\{\nabla u^T - (\overline{p}_T, \overline{q}_T)\right\}\cdot\mathbf{n}_j^T\right]$$

Damping term

This becomes the Galerkin scheme for $\alpha = 2$ (See Nishikawa JCP2007)

- **LDA Scheme (Upwind):** Very accurate scheme. Details in the paper.

We now have good diffusion schemes for residual-distribution method!

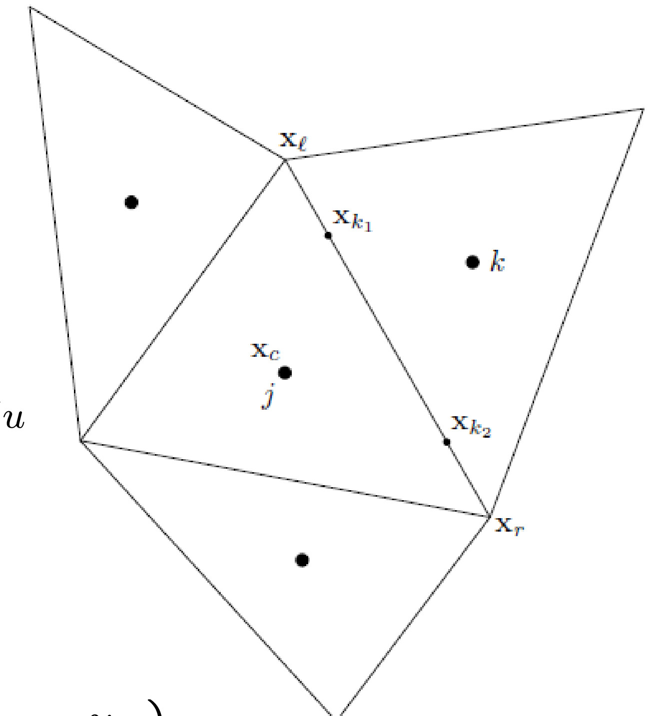
Discontinuous Galerkin Schemes

$$u_j(x,y) = \overline{u}_j + \psi_1 \overline{\partial_x u}_j + \psi_2 \overline{\partial_y u}_j$$

Derived diffusion scheme:

$$V_j \frac{d\overline{u}_j}{dt} = -\int_{\partial T_j} (f,g)\cdot \hat{\mathbf{n}} dA$$

$$\begin{bmatrix} \dfrac{d\left(\overline{\partial_x u_j}\right)}{dt} \\ \dfrac{d\left(\overline{\partial_y u_j}\right)}{dt} \end{bmatrix} = M_j^{-1} \begin{bmatrix} -\int_{\partial T_j} \psi_1 (f,g)\cdot \hat{\mathbf{n}} dA + \int_{T_j} \nabla\psi_1 \cdot (f,g), \\ -\int_{\partial T_j} \psi_2 (f,g)\cdot \hat{\mathbf{n}} dA + \int_{T_j} \nabla\psi_2 \cdot (f,g) \end{bmatrix}$$



Volume Integral: Integration by parts with $(f,g) = -\nu \nabla u$

$$\int_{T_j} \nabla\psi_1 \cdot (f,g) = -\nu \oint_{\partial T_j} u \nabla\psi_1 \cdot \hat{\mathbf{n}}_k dA_k - \int_{T_j} u \nabla^2 \psi_1$$

Diffusive flux derived from the upwind flux:

$$\phi_k(\mathbf{x}_{k_n}) = -\frac{\nu}{2}\left[\, \nabla u_j + \nabla u_k \,\right]\cdot \hat{\mathbf{n}}_k - \frac{\nu\alpha}{2L_r}(u_R - u_L)$$

Consistent part **Damping term (skewness measure)**

The DG diffusion scheme is nice and compact: involves only neighbors.

Spectral-Volume Scheme

Spectral-volume (SV) scheme:

Polynomial reconstruction over a spectral volume:

$$u_T(x,y) = \sum_{i \in \{C_T\}} u_i L_i(x,y)$$

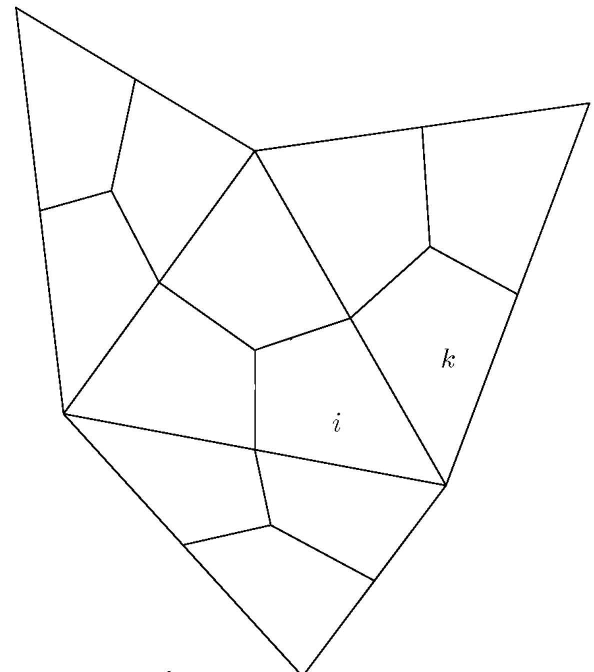
$$\frac{1}{V_i}\int_{C_i} u_T \, dV = u_i$$

Derived diffusion scheme:

$$\frac{du_i}{dt} = -\frac{1}{V_i}\sum_{k \in \{K_i\}} \phi_{ik} A_k$$

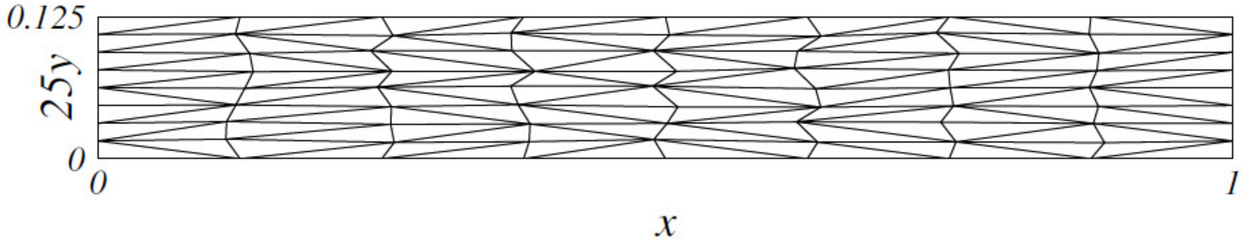
$$\phi_{jk} = -\frac{\nu}{2}\left[\, \nabla u_T + \nabla u_{T_k} \,\right] \cdot \hat{\mathbf{n}}_k - \frac{\nu\alpha}{2L_r}(u_R - u_L)$$

Consistent part **Damping term (skewness measure)**



SV scheme is nice and simple; no volume integrals required.

Test Problem – Highly-Skewed Grids



Problem:

$$u_t = \nu(u_{xx} + u_{yy})$$

$$u(x, y, 0) = 5\sin(\pi x)\sin(4000\pi y)$$

Compute the solution at t =1.0e-08

Irregular Grids: 25x25, 33x33, …, 129x129, 137x137 (15 grids)

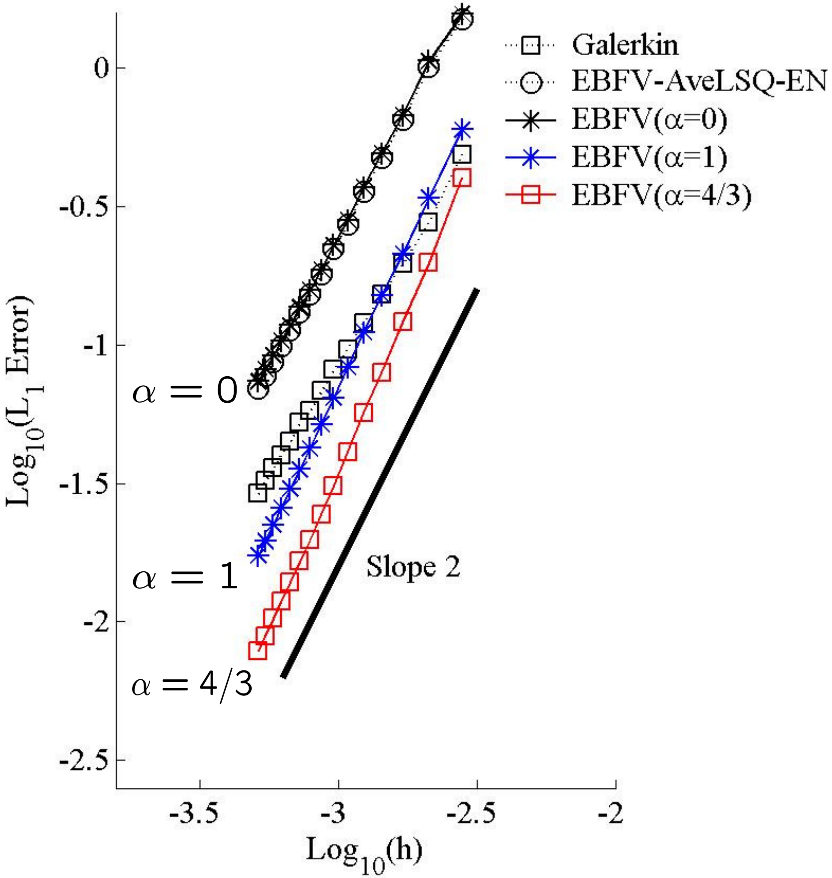
Global time step (the forward-Euler explicit):

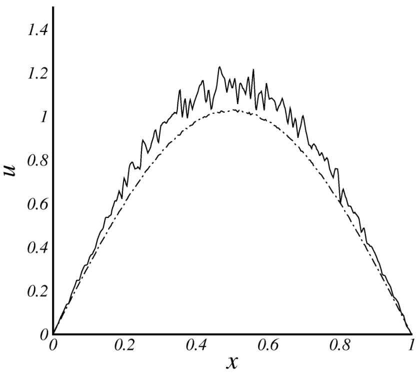
$$\Delta t = 0.003\, h^2$$

Total time steps = 77, 137, 214, 308, 419, 547, 692, 854, 1033, 1229, 1443, 1673, 1921, 2185, 2467.

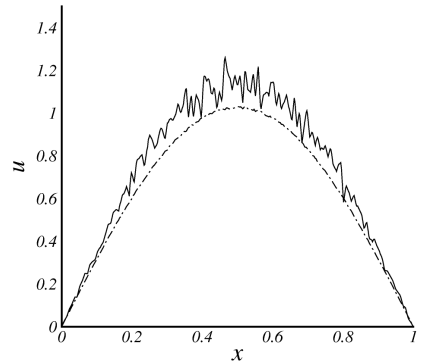
Compute the error at the data point at the final time.

Results for EBFV Schemes

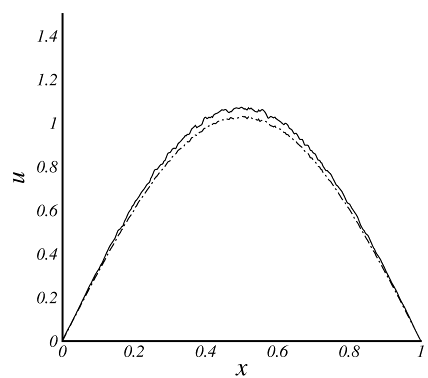




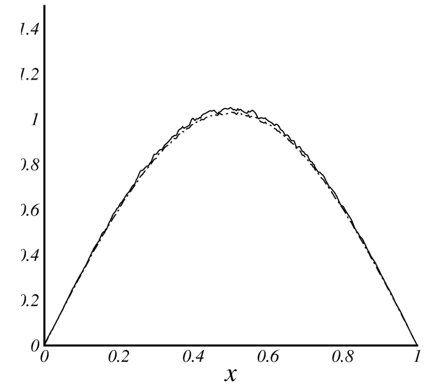
Avg-LSQ-EN



EBS(α =0)



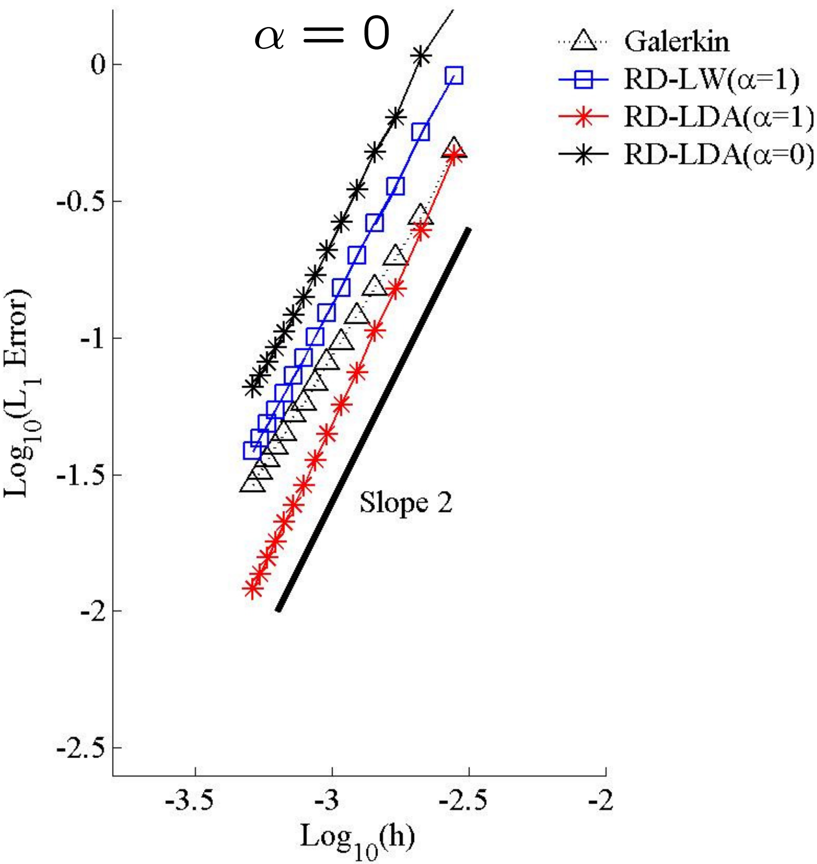
EBS(α =1)

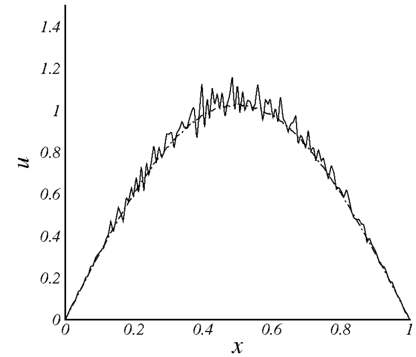


EBS(α =4/3)

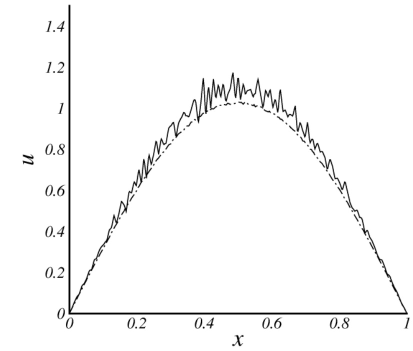
Lack of damping → Large error, Oscillations

Results for RD Schemes

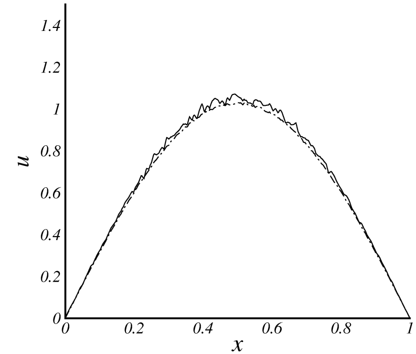




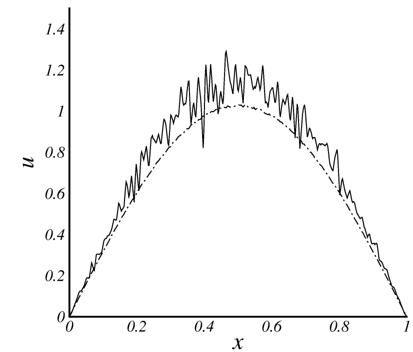
Galerkin



LW (α =1)



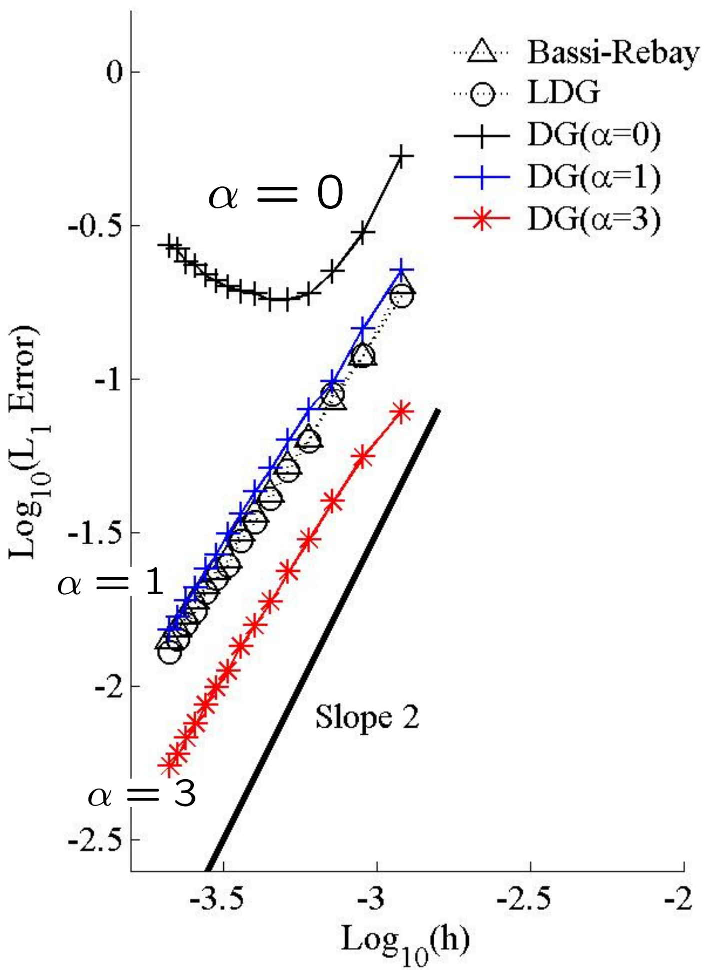
LDA (α =1)

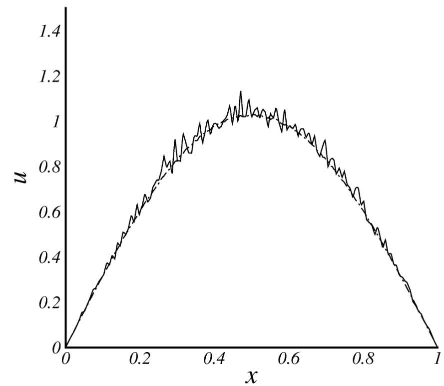


LDA (α =0)

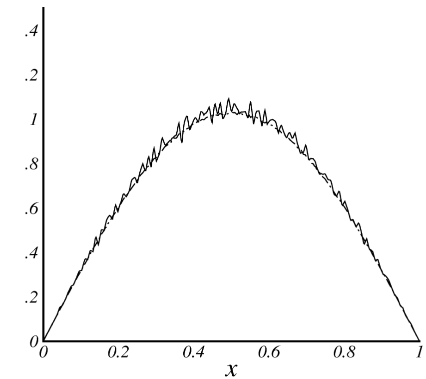
Lack of damping -> Large error and oscillations

Results for DG Schemes

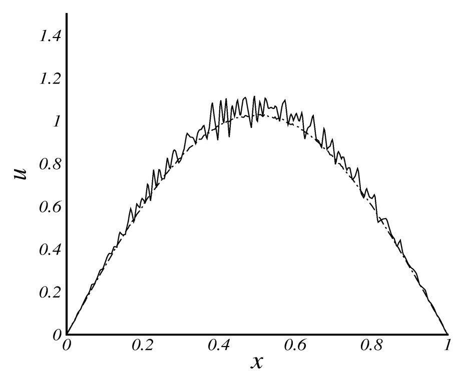




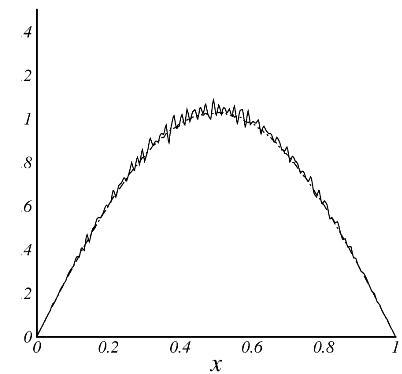
Bassi-Rebay



LDG



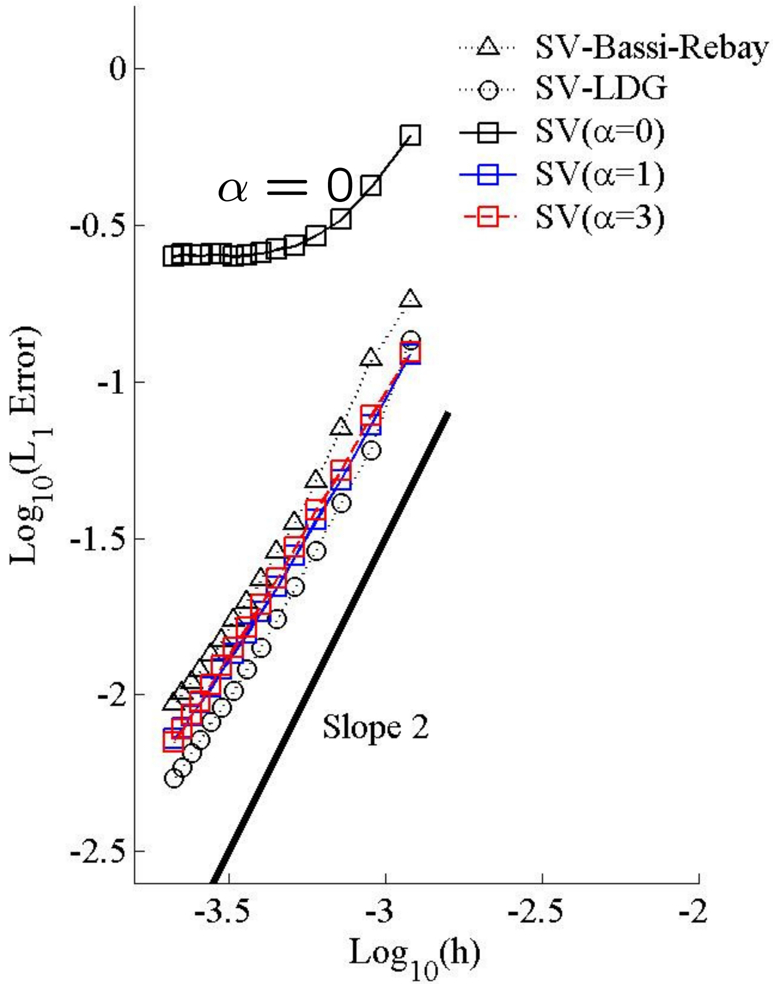
DG(α =1)

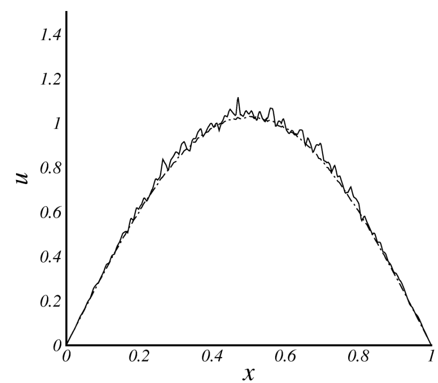


DG(α =3)

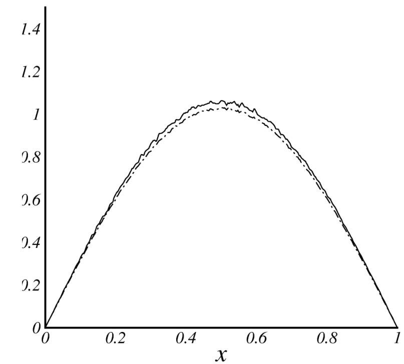
Lack of damping -> Inconsistent, unstable, highly oscillatory

Results for SV Schemes

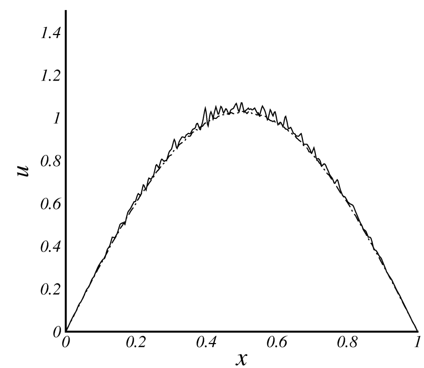




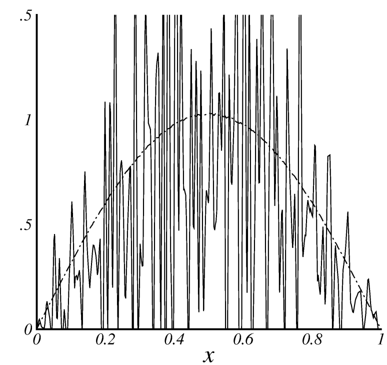
Bassi-Rebay



LDG



SV(α =1)



SV(α =0)

Lack of damping -> Inconsistent, unstable, highly oscillatory

Future Work

Three dimensions – *straightforward*

Advection-diffusion – *remarkably simple*

Higher-order schemes – *just try them*

Nonlinear systems – *2 strategies*

1. Interface gradient: $\phi_k \;=\; -\nu \, \nabla u|_k \cdot \hat{\mathbf{n}}_k$

$$\nabla u|_k = \frac{1}{2}\left[\, \overline{\nabla u_j} + \overline{\nabla u_k} \,\right] + \frac{\alpha}{2L_r}(u_R - u_L)\hat{\mathbf{n}}_k$$

2. Follow the principle