First, Second, and Third Order Finite-Volume Schemes for Diffusion

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All Created Equal

“all men are created equal,”

- Thomas Jefferson, The Declaration of Independence

Are all PDEs created equal?

Hyperbolic vs Parabolic

Hyperbolic (inviscid):

- *Principle of "upwinding" (dissipation) led to many useful schemes.*
- *Robust 1st-order schemes - a home to come back.*
- *A variety of unstructured, high-order schemes.*

Parabolic (viscous):

- *Lack of universal guiding principles.*
- *Lack of robust 1st-order schemes (rely on inconsistent scheme).*
- *Much less variety for unstructured, high-order schemes.*
- *Degraded accuracy of derivatives on irregular grids.*

They don't seem created equal...

Who Created PDEs?

"all men are created equal, that they are endowed by their Creator with certain unalienable Rights,"

-Thomas Jefferson, The Declaration of Independence

We created PDEs.

Then, we can recreate them equal.

Recreate Them Hyperbolic

First-Order Hyperbolic System Method

JCP2007, 2010, 2012, AIAA2009, 2011, 2013

$$\mathbf{U}_t + \mathbf{A}\mathbf{U}_x = \mathbf{B}\mathbf{U}_{xx} + \mathbf{C}\mathbf{U}_{xxx} + \cdots + \mathbf{S}$$

$$\Downarrow$$

$$\tilde{\mathbf{W}}_t + \tilde{\mathbf{A}}\tilde{\mathbf{W}}_x = 0$$

Methods for hyperbolic systems apply to all PDEs.

Dramatic simplification/improvements to numerical methods

Turn Every Food into a Burger

Simple, Efficient, Accurate.

Sushi Burger!

It looks eccentric, but the taste is the same, or even better.

Nishikawa, JCP2007

Hyperbolic Diffusion System

$$\partial_t u = \nu\,(\partial_{xx} u + \partial_{yy} u)$$

Sushi Burger for Diffusion

steady

$$\begin{aligned} \cancel{\partial_t u} &= \nu\,(\partial_x p + \partial_y q) \\ \cancel{\partial_t p} &= (\partial_x u - p)/T_r \\ \cancel{\partial_t q} &= (\partial_y u - q)/T_r \end{aligned} \rightarrow \begin{aligned} 0 &= \nu\,(\partial_x p + \partial_y q), \\ p &= \partial_x u, \\ q &= \partial_y u, \end{aligned} \rightarrow \quad 0 = \nu\,(\partial_{xx} u + \partial_{yy} u),$$

System is equivalent to diffusion in the steady state for *any Tr* :

$$T_r = \frac{L_r^2}{\nu}, \quad L_r = \frac{1}{2\pi}$$

Unsteady computation possible by dual-time formulation (implicit) with a steady solver used in the inner iteration.

Nishikawa, JCP2007

Hyperbolic Diffusion System

Sushi Burger for Diffusion

$$\partial_t \mathbf{U} + \partial_x \mathbf{F} + \partial_y \mathbf{G} = \mathbf{S},$$

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

Normal Jacobian: $\mathbf{A}_n = \dfrac{\partial \mathbf{H}}{\partial \mathbf{U}} = \dfrac{\partial(\mathbf{F}n_x + \mathbf{G}n_y)}{\partial \mathbf{U}}$

Real eigenvalues: $\lambda_1 = -\sqrt{\dfrac{\nu}{T_r}}, \quad \lambda_2 = \sqrt{\dfrac{\nu}{T_r}}, \quad \lambda_3 = 0$

Energy Estimate

Integrate over the domain $\ell^E = (u,\, L_r^2 p,\, L_r^2 q)$ x (hyperbolic system):

steady

$$\frac{d}{dt}\int_\Omega E\,dV = -\nu\int_\Omega (p^2+q^2)\,dV - \oint_{\partial\Omega} \mathbf{f}^E\cdot\mathbf{n}\,dA$$

$E = u^2 + L_r^2(p^2+q^2)$

$\mathbf{f}^E = (-\nu u p, -\nu u q)$

which reduces to the energy estimate for the Laplace equation:

$$0 = \int_\Omega \nabla u\cdot\nabla u\,dV - \oint_{\partial\Omega} u\frac{\partial u}{\partial n}dA$$

Energy estimate consistent with steady diffusion problem

Diffusion is Hyperbolic

Hyperbolic Advection-Diffusion System (JCP2010)
Hyperbolic Navier-Stokes System (AIAA2011-3043)

If you have a good inviscid scheme,
you have a very good viscous scheme.

- Equal order of accuracy for solution and derivatives.
- O(h) time step; O(1/h) condition number.

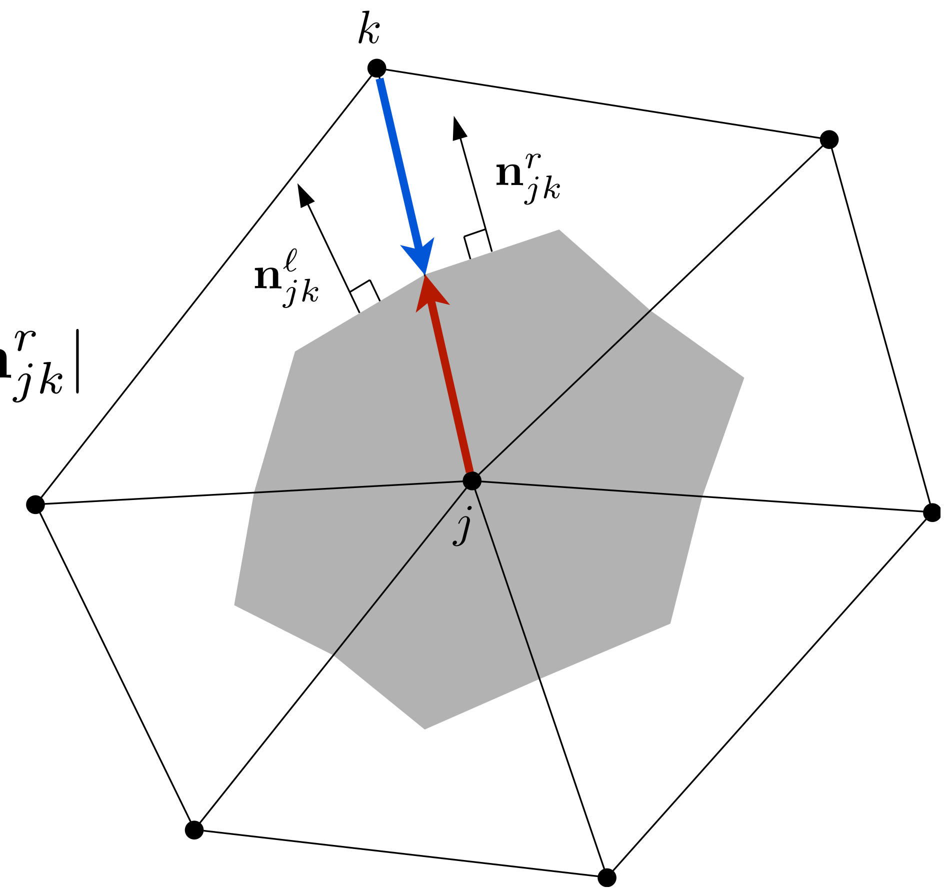
Edge-Based Finite-Volume Method

NASA's FUN3D; Software Cradle's SC/Tetra; DLR Tau code, etc.

Edge-based finite-volume scheme:

$$V_j \frac{d\mathbf{U}_j}{dt} = -\sum_{k\in\{k_j\}} \Phi_{jk} A_{jk} + \mathbf{S}_j V_j$$

$$A_{jk} = |\mathbf{n}_{jk}^{\ell} + \mathbf{n}_{jk}^{r}|$$



with the upwind flux at edge midpoint:

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

Accuracy is determined by the left and right states.

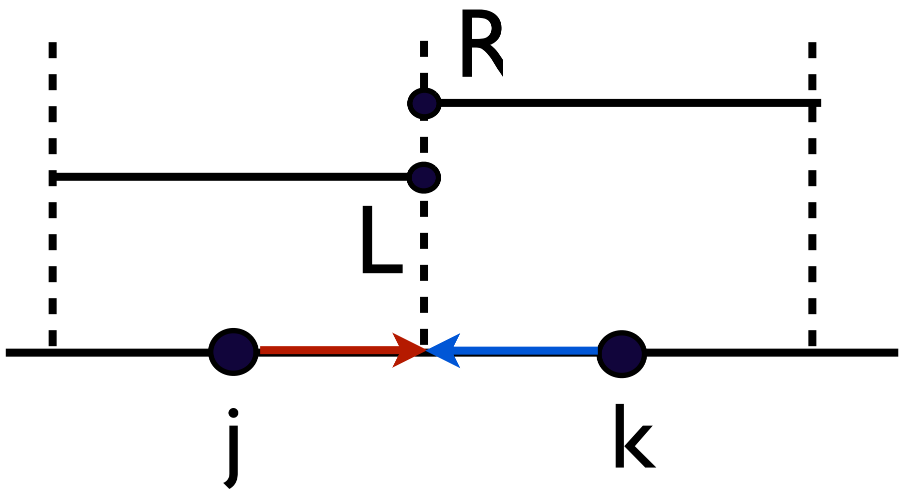
First-Order Scheme

Home sweet home for diffusion schemes

First-Order Scheme for Diffusion

Left and right states:

$$\mathbf{U}_L = \mathbf{U}_j, \quad \mathbf{U}_R = \mathbf{U}_k$$



Discrete Energy Estimate:

$$\underbrace{\sum_{j\in\{j\}} V_j \frac{dE_j}{dt} = -\sum_{e_b\in\{e_b\}} \frac{\mathbf{f}_1^E + \mathbf{f}_2^E}{2}\hat{\mathbf{n}}_{e_b} A_{e_b} - \sum_{j\in\{j\}} \nu(p_j^2 + q_j^2)V_j}_{\text{Consistent with continuous energy estimate}} \underbrace{\boxed{-\frac{\nu}{2L_r}\sum_{e\in\{e\}} \epsilon_{jk} A_{jk}}}_{\text{Dissipation}}$$

$$\epsilon_{jk} = (u_k - u_j)^2 + L_r^2\left[(p_k - p_j, q_k - q_j)\cdot\hat{\mathbf{n}}_{jk}\right]^2 \geq 0$$

First-order upwind diffusion scheme is energy-stable for general grids.

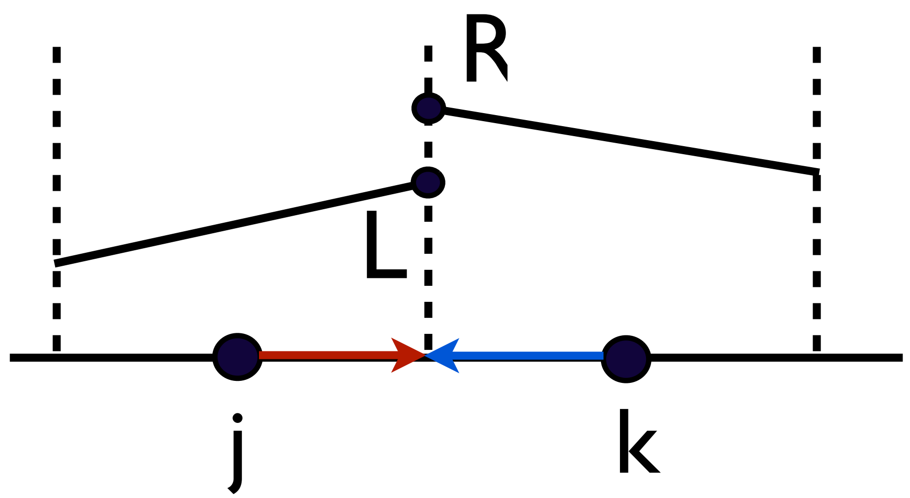
Second-Order Scheme

Even better

Second-Order Scheme

For triangular/tetrahedral and smooth mixed grids.

1. Compute gradients at nodes (e.g., LSQ).
2. Extrapolate the solution to the midpoint.



Left and right states:

$$u_L = u_j + \frac{1}{2}\boxed{(p_j, q_j)} \cdot \Delta \mathbf{l}_{jk}, \quad u_R = u_k - \frac{1}{2}\boxed{(p_k, q_k)} \cdot \Delta \mathbf{l}_{jk}$$

$$p_L = p_j + \frac{1}{2} \nabla p_j \cdot \Delta \mathbf{l}_{jk}, \quad p_R = p_k - \frac{1}{2} \nabla p_k \cdot \Delta \mathbf{l}_{jk}$$

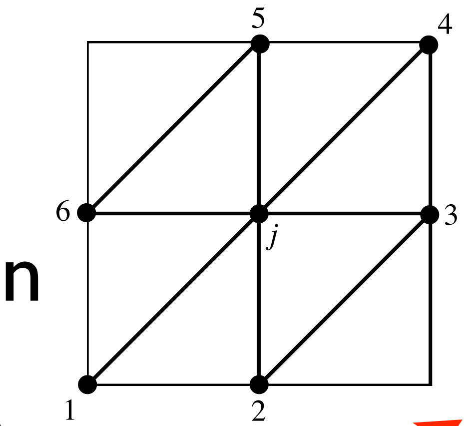
$$q_L = q_j + \frac{1}{2} \nabla q_j \cdot \Delta \mathbf{l}_{jk}, \quad q_R = q_k - \frac{1}{2} \nabla q_k \cdot \Delta \mathbf{l}_{jk}$$

$$\Delta \mathbf{l}_{jk} = (x_k - x_j, y_k - y_j)$$

Gradients are not needed for the solution.

Taylor Expansion

Source discretization



steady

$$\frac{du_j}{dt} = \nu(\partial_x p + \partial_y q) - \frac{\nu h}{6L_r}\left[(\sqrt{2}+\sqrt{5})\partial_x(p-\partial_x u) + \sqrt{2}\partial_y(p-\partial_x u) + \sqrt{2}\partial_x(q-\partial_y u) + (\sqrt{2}+\sqrt{5})\partial_y(q-\partial_y u)\right] - \frac{\nu h^2}{12}\left[\partial_{xx}(\partial_x p + \partial_y q) + \partial_{xy}(\partial_x p + \partial_y q) + \partial_{yy}(\partial_x p + \partial_y q)\right] + \boxed{O(h^3)},$$

steady

$$\frac{dp_j}{dt} = \frac{1}{T_r}(\partial_x u - p) - \boxed{\frac{h^2}{6T_r}\left[\partial_{xx}(p-\partial_x u) + \partial_{xy}(p-\partial_x u) + \partial_{xy}(q-\partial_y u) + \frac{1}{2}(\partial_{xx}p + \partial_{yy}p + \partial_{xx}q)\right]} + O(h^3),$$

steady

$$\frac{dq_j}{dt} = \frac{1}{T_r}(\partial_y u - q) - \boxed{\frac{h^2}{6T_r}\left[\partial_{yy}(q-\partial_y u) + \partial_{xy}(q-\partial_y u) + \partial_{xy}(p-\partial_x u) + \frac{1}{2}(\partial_{xx}q + \partial_{yy}q + \partial_{xx}p)\right]} + O(h^3)$$

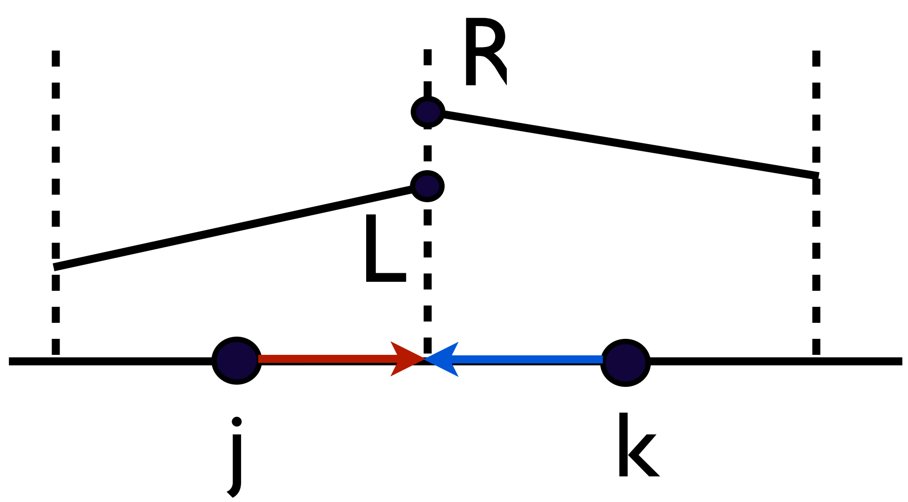
Second-order accurate for solution and gradients.
First-order error makes it stable with forward Euler.

Third-Order Scheme

A new wave

Third-Order Scheme (Katz and Sankaran JCP2011)

For triangular/tetrahedral grids only.



1. 2nd-order gradients at nodes (e.g., LSQ quadratic fit).

2. Extrapolate flux/solution to the midpoint.

$$\mathbf{H}_L = \mathbf{H}_j + \frac{1}{2}\nabla\mathbf{H}_j \cdot \Delta\mathbf{l}_{jk}, \quad \mathbf{H}_R = \mathbf{H}_k - \frac{1}{2}\nabla\mathbf{H}_k \cdot \Delta\mathbf{l}_{jk}$$

Third-order accuracy on a second-order stencil

Source term needs special discretization (NIA CFD Seminar 12-04-12).

Divergence Form of Source

Write the source term at each node j as follows:

$$\mathbf{S} \longrightarrow \partial_x \mathbf{F}^s + \partial_y \mathbf{G}^s$$

$$\mathbf{F}^s = \begin{bmatrix} 0 \\ (y - y_j)\, q/T_r \\ -(x - x_j)\, q/T_r \end{bmatrix}, \quad \mathbf{G}^s = \begin{bmatrix} 0 \\ -(y - y_j)\, p/T_r \\ (x - x_j)\, p/T_r \end{bmatrix}$$

So that

$$\partial_t \mathbf{U} + \partial_x \mathbf{F} + \partial_y \mathbf{G} = \mathbf{S}$$

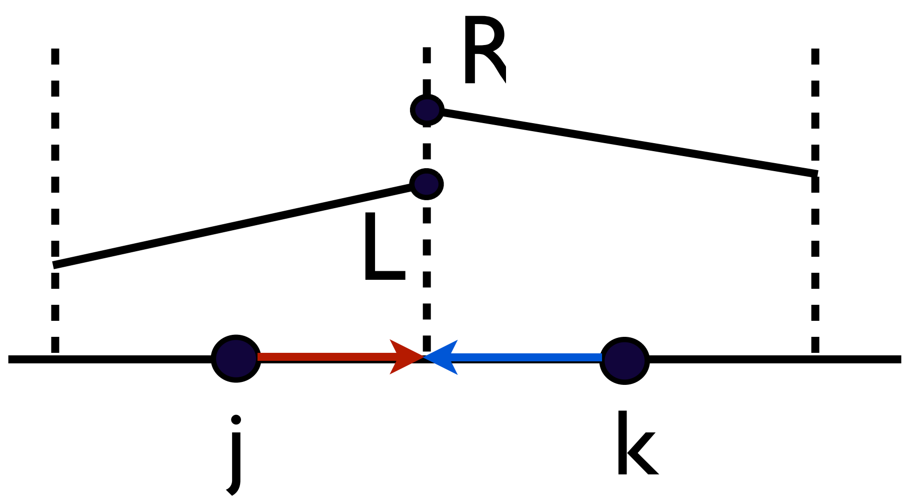
$$\downarrow$$

$$\partial_t \mathbf{U} + \partial_x (\mathbf{F} - \mathbf{F}^s) + \partial_y (\mathbf{G} - \mathbf{G}^s) = \mathbf{0}$$

The system is fully hyperbolic with no source terms.
Source term discretization is not needed.

Third-Order Scheme (Katz and Sankaran JCP2011)

1. 2nd-order gradients at nodes (e.g., LSQ).
2. Extrapolate flux/solution to the midpoint.
3. Upwind flux for fully hyperbolic system.



Left and right states:

$$u_L = u_j + \frac{1}{2}\boxed{(p_j, q_j)} \cdot \Delta \mathbf{l}_{jk}, \quad u_R = u_k - \frac{1}{2}\boxed{(p_k, q_k)} \cdot \Delta \mathbf{l}_{jk}$$

$$p_L = p_j + \frac{1}{2}\nabla p_j \cdot \Delta \mathbf{l}_{jk}, \quad p_R = p_k - \frac{1}{2}\nabla p_k \cdot \Delta \mathbf{l}_{jk}$$

$$q_L = q_j + \frac{1}{2}\nabla q_j \cdot \Delta \mathbf{l}_{jk}, \quad q_R = q_k - \frac{1}{2}\nabla q_k \cdot \Delta \mathbf{l}_{jk}$$

Gradients are not needed for the solution.

Taylor Expansion (3rd-order)

steady

$$\cancel{\frac{du_j}{dt}} = \nu(\cancel{\partial_x p + \partial_y q})$$
$$- \frac{\nu h}{6L_r}\left[(\sqrt{2}+\sqrt{5})\partial_x(\cancel{p - \partial_x u}) + \sqrt{2}\partial_y(\cancel{p - \partial_x u}) + \sqrt{2}\partial_x(\cancel{q - \partial_y u}) + (\sqrt{2}+\sqrt{5})\partial_y(\cancel{q - \partial_y u})\right]$$
$$- \frac{\nu h^2}{12}\left[\partial_{xx}(\cancel{\partial_x p + \partial_y q}) + \partial_{xy}(\cancel{\partial_x p + \partial_y q}) + \partial_{yy}(\cancel{\partial_x p + \partial_y q})\right] + \boxed{O(h^3),}$$

steady

$$\cancel{\frac{dp_j}{dt}} = \frac{1}{T_r}(\cancel{\partial_x u - p}) - \frac{h^2}{6T_r}\left[(\partial_{xx} + \partial_{xy})(\cancel{q - \partial_y u}) + \partial_{xx}(\cancel{p - \partial_x u}) + \partial_y(\cancel{\partial_x q - \partial_y p})\right] + \boxed{O(h^3),}$$

steady

$$\cancel{\frac{dq_j}{dt}} = \frac{1}{T_r}(\cancel{\partial_y u - q}) - \frac{h^2}{6T_r}\left[(\partial_{xy} + \partial_{yy})(\cancel{p - \partial_x u}) + \partial_{yy}(\cancel{q - \partial_y u}) - \partial_x(\cancel{\partial_x q - \partial_y p})\right] + \boxed{O(h^3)}$$

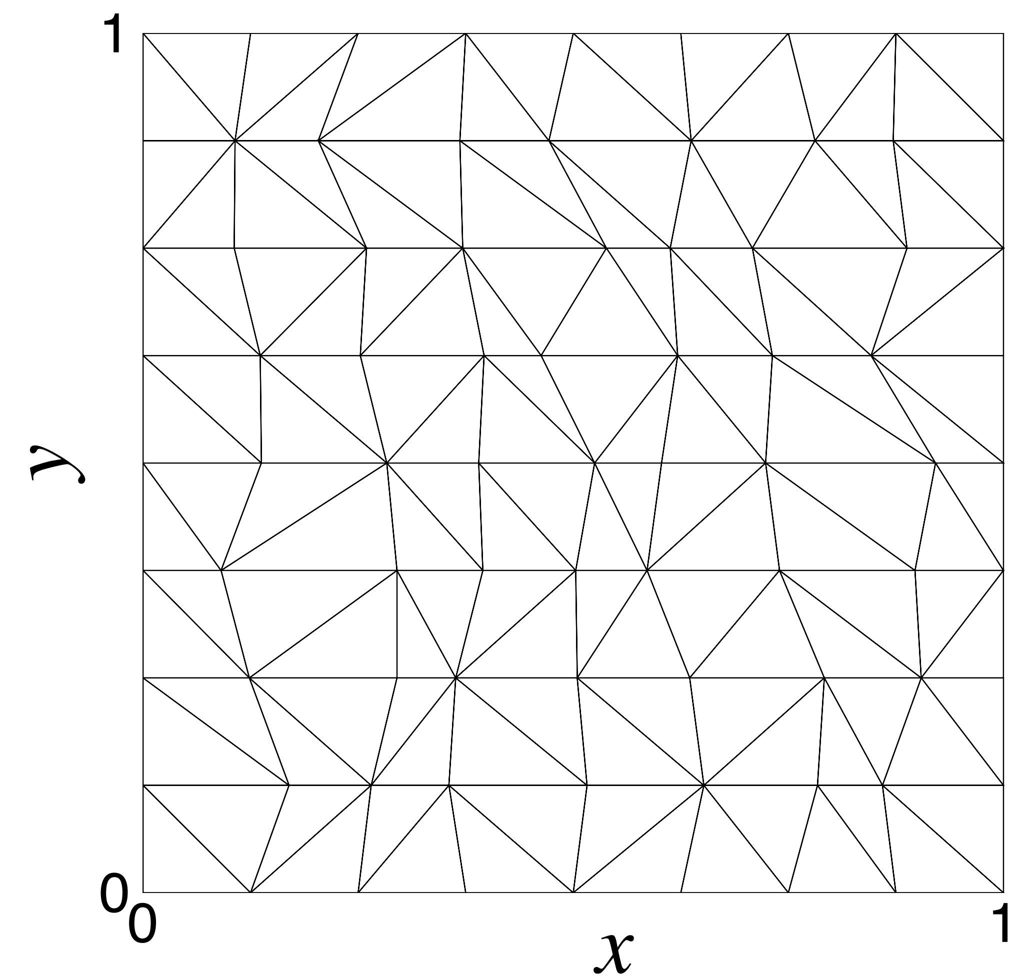
Third-order accurate for solution and gradients.

First-order error makes it stable with forward Euler.

Numerical Experiment

Exact solution:

$$u(x,y) = \frac{\sinh(\pi x)\sin(\pi y) + \sinh(\pi y)\sin(\pi x)}{\sinh(\pi)}$$



- n x n grids: n = 9, 17, 33, 65, 129, 257.

- Dirichlet boundary condition.

- 10 neighbors for quadratic fit.
  (to avoid ill-conditioning of LSQ matrix)

- Forward Euler time stepping

- Steady state reached when residual drops below 1.0E-15

- Comparison with the Galerkin scheme

Max CFL Number

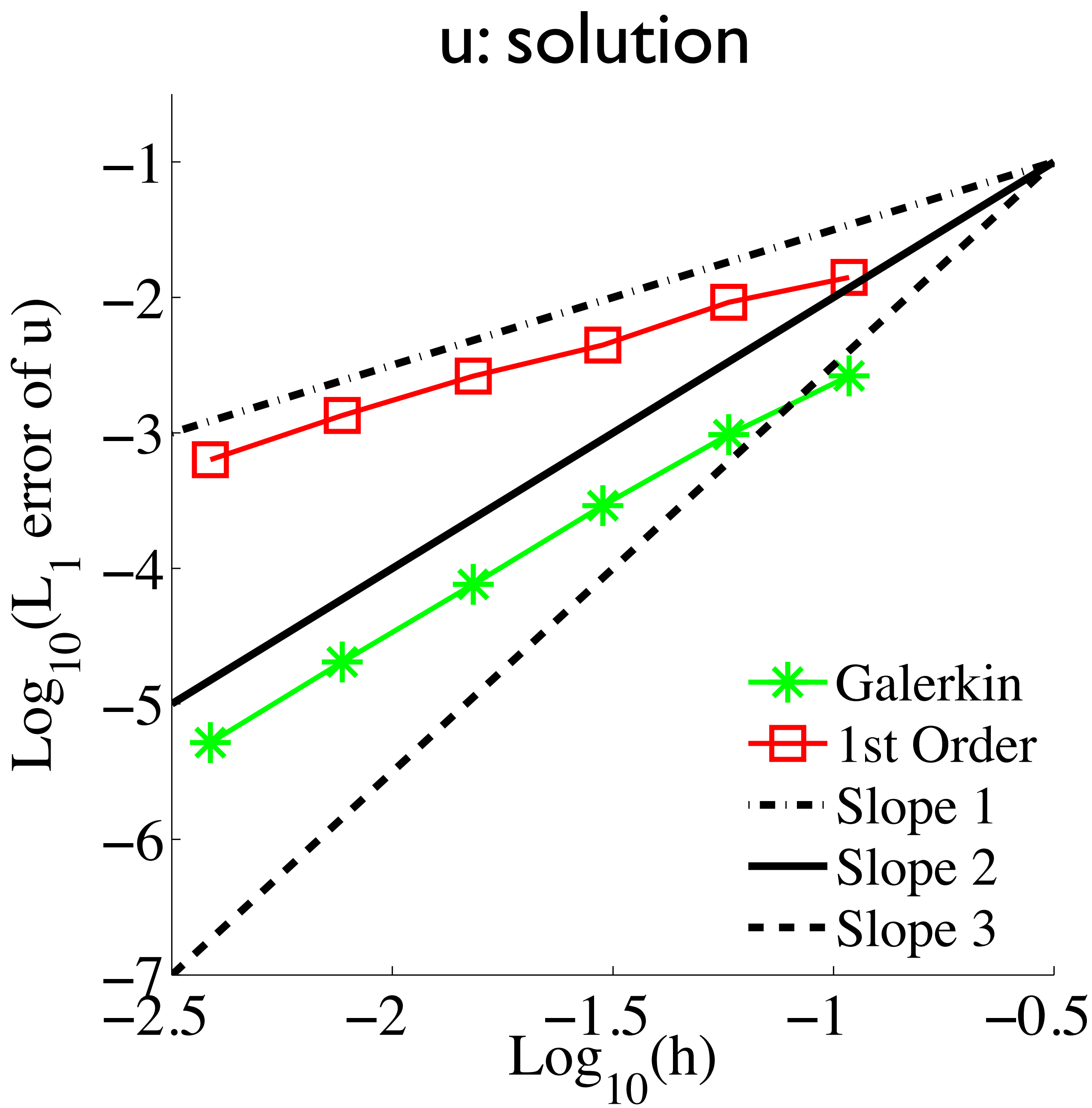
Max CFL numbers determined by Fourier analysis:

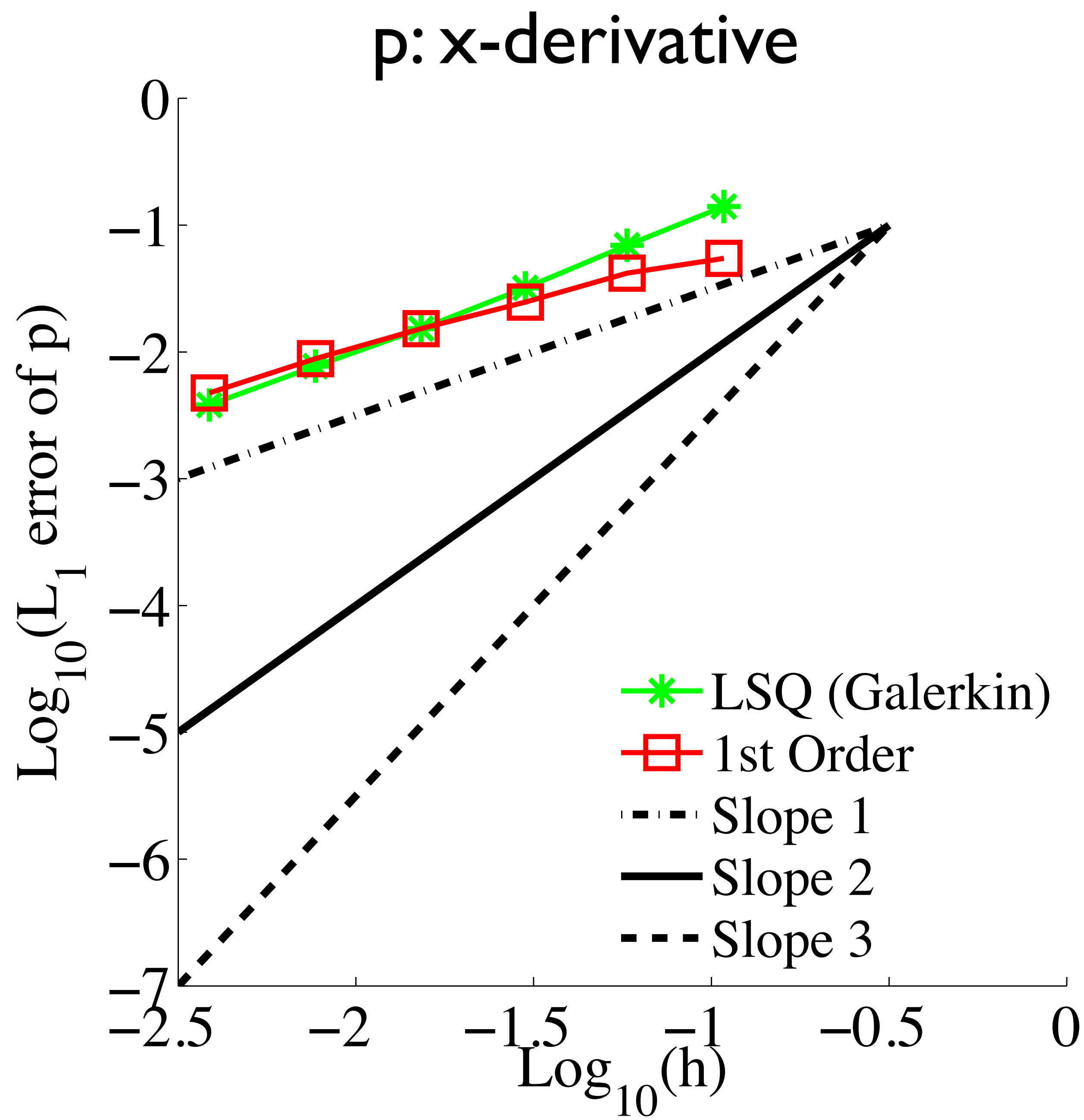
	First-Order	Second-Order	Third-Order
Forward Euler	1.3032	0.7313	0.7313

Hyperbolic schemes are stable with O(h) time step:

O(1/h) faster than typical schemes with O(h^2) time step.

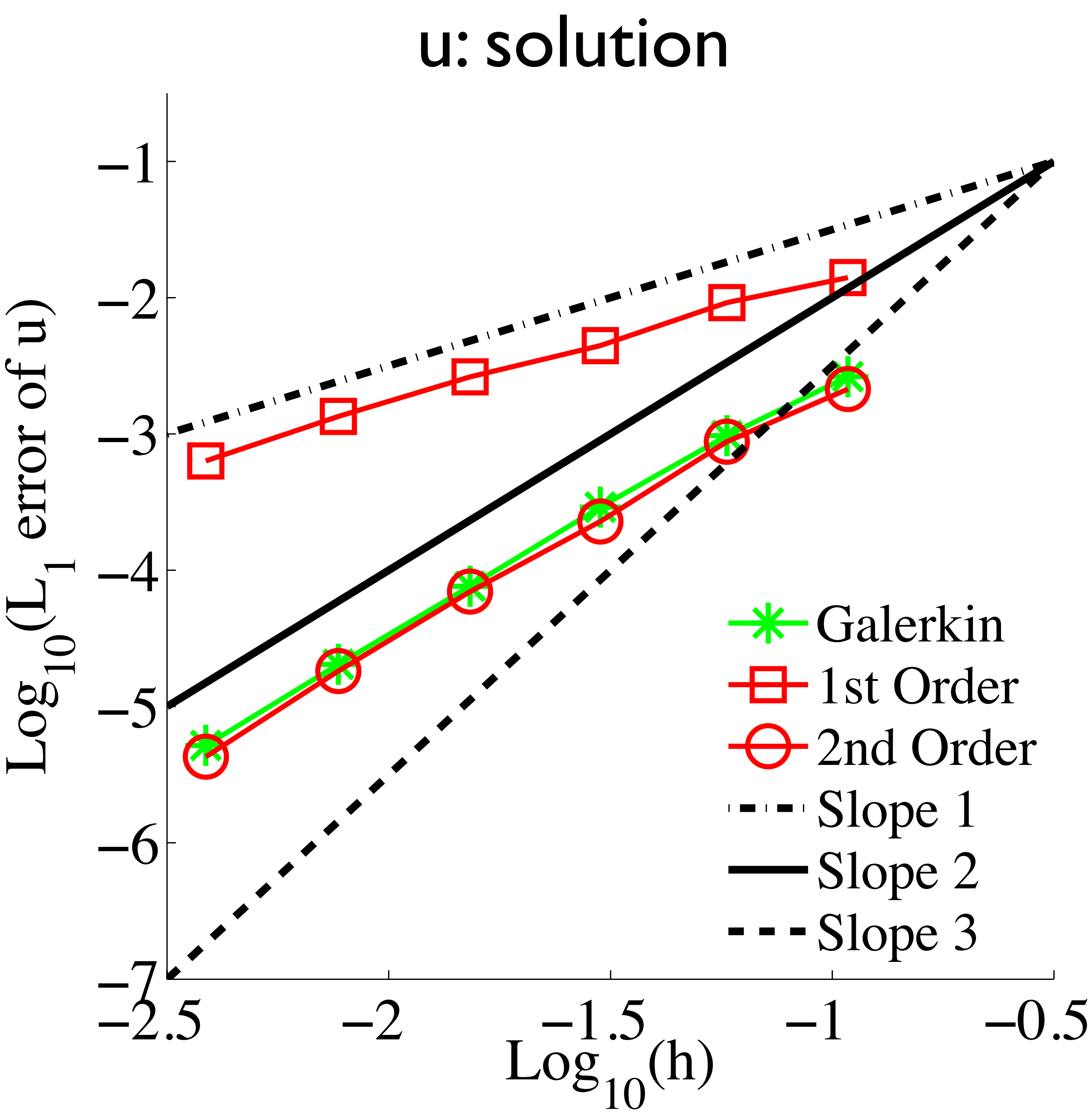
Error Convergence 1

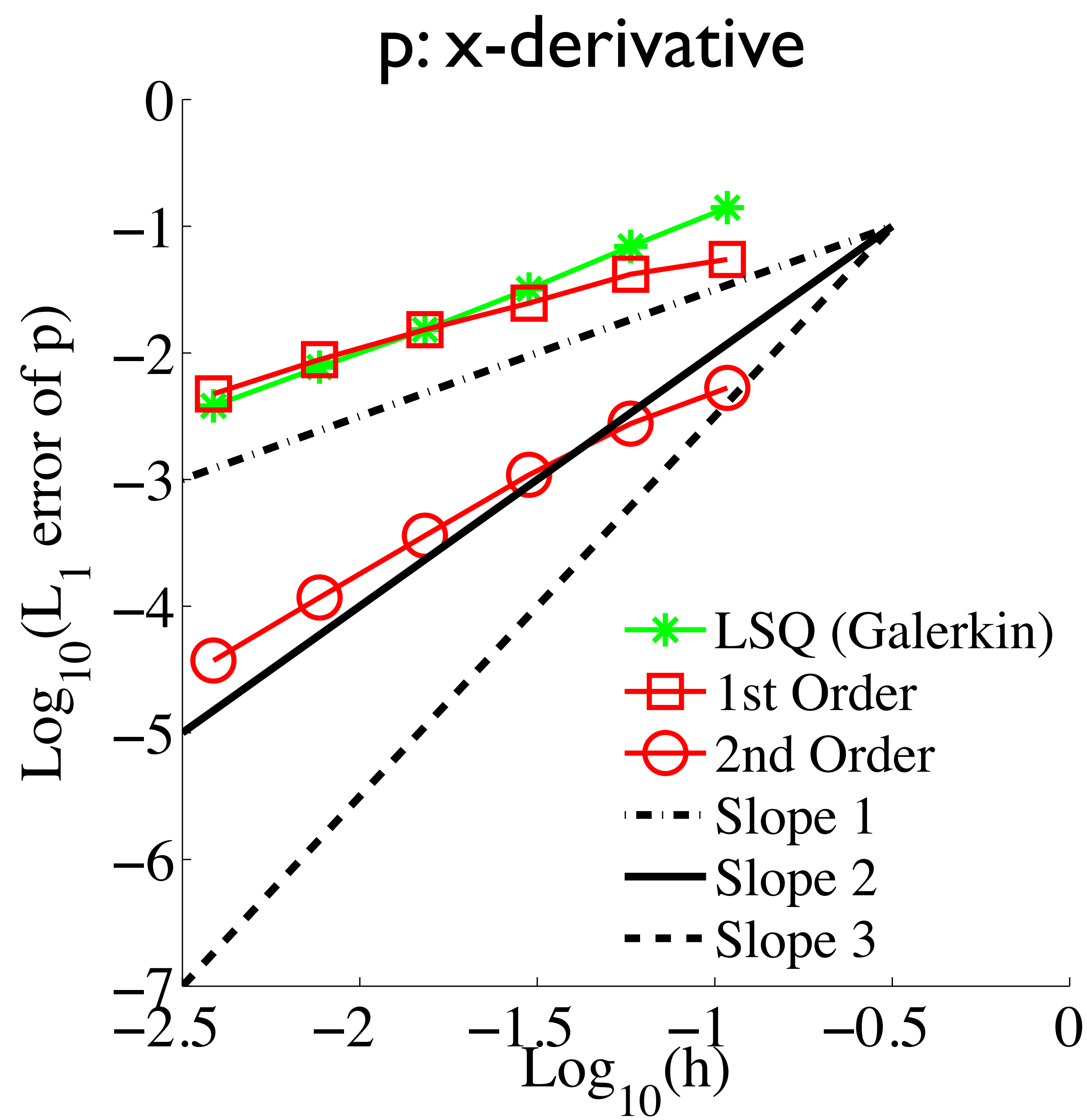




1st-order accurate solution and gradients.

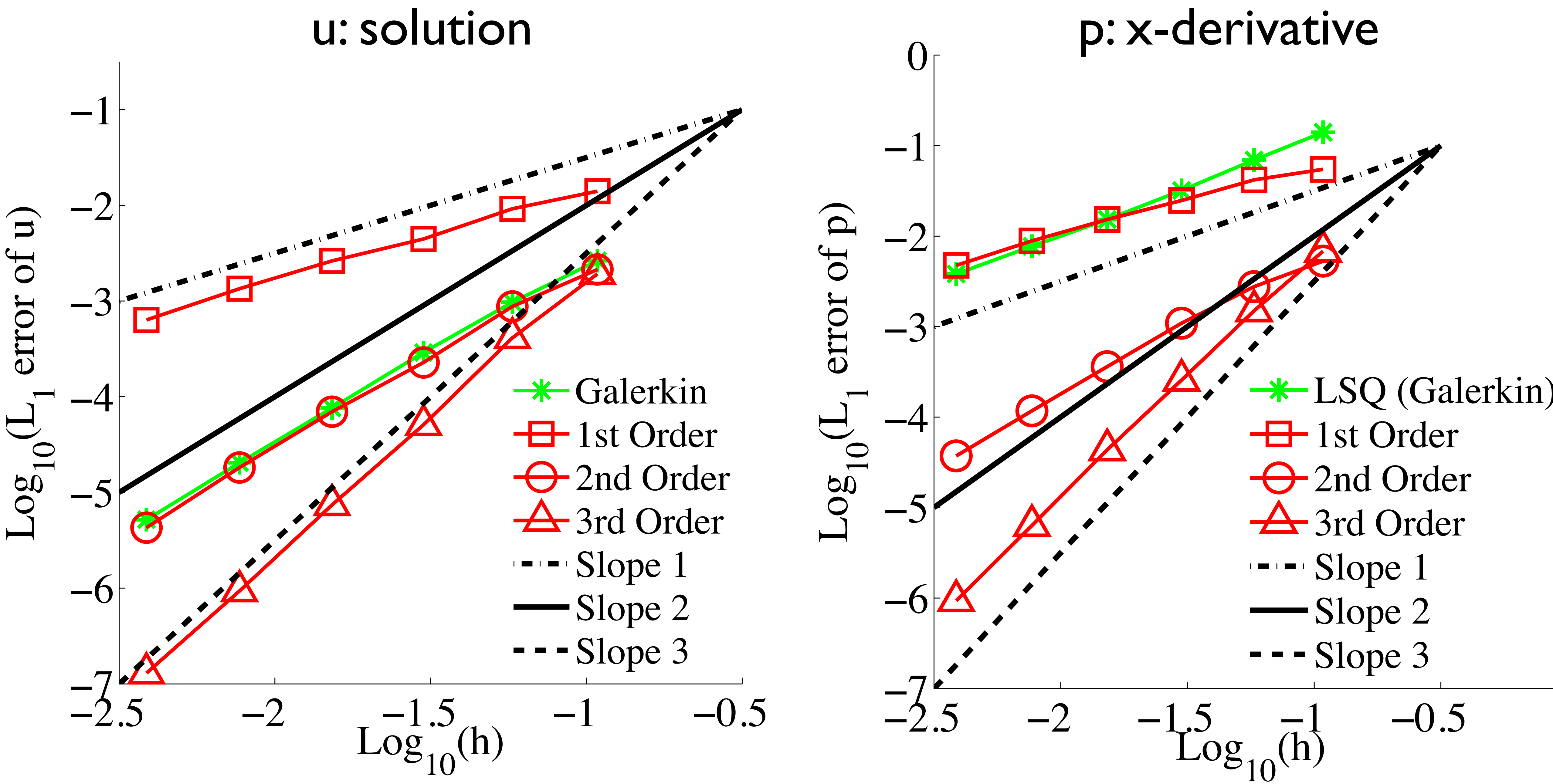
Error Convergence 2





2nd-order accurate solution and gradients.

Error Convergence 3



3rd-order accurate solution and gradients.

Cost Comparison

Cost per time step (the irregular grid case).

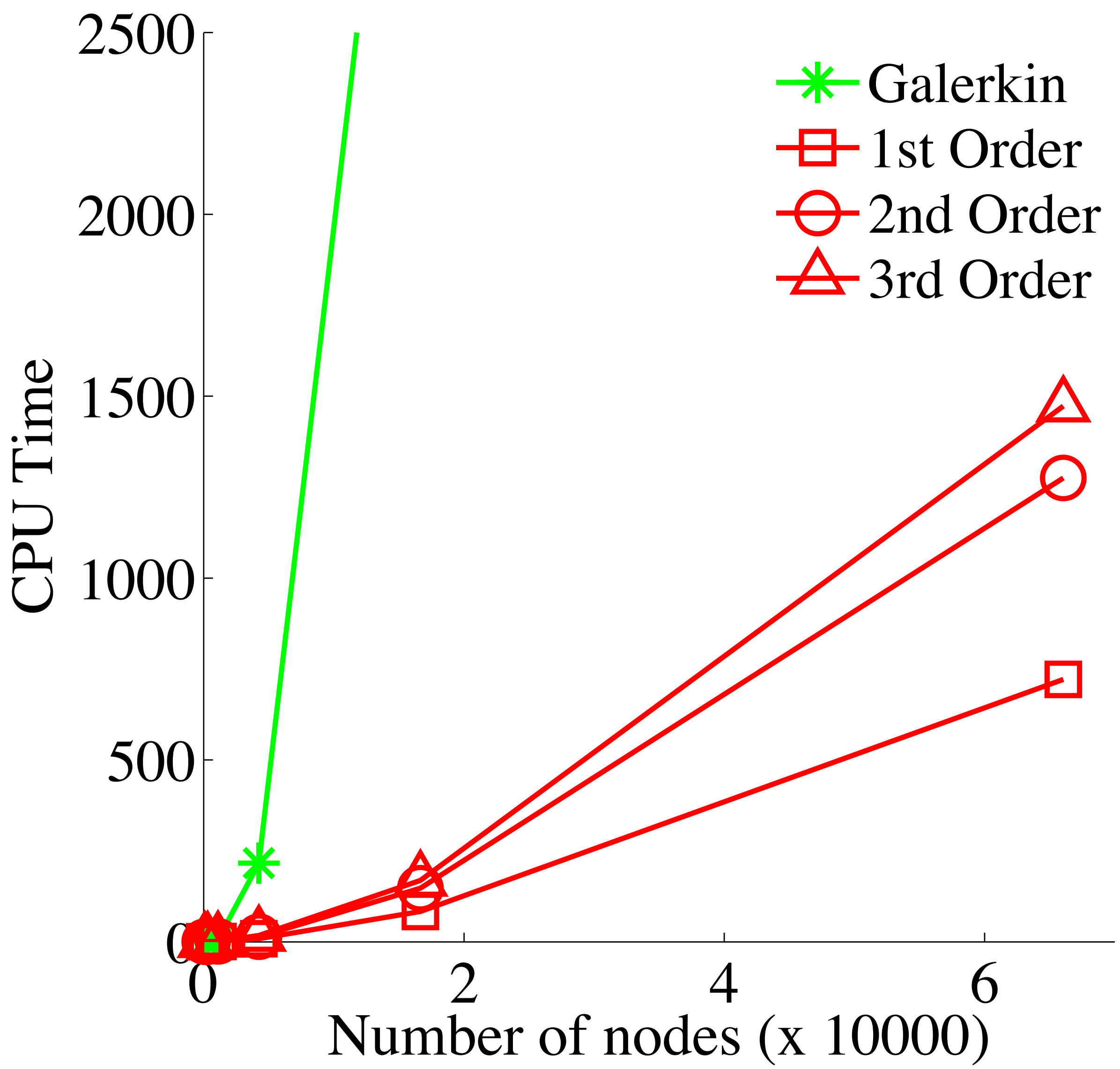
	Galerkin	First-Order	Second-Order	Third-Order
Forward Euler	0.66	1.00	1.26	1.33

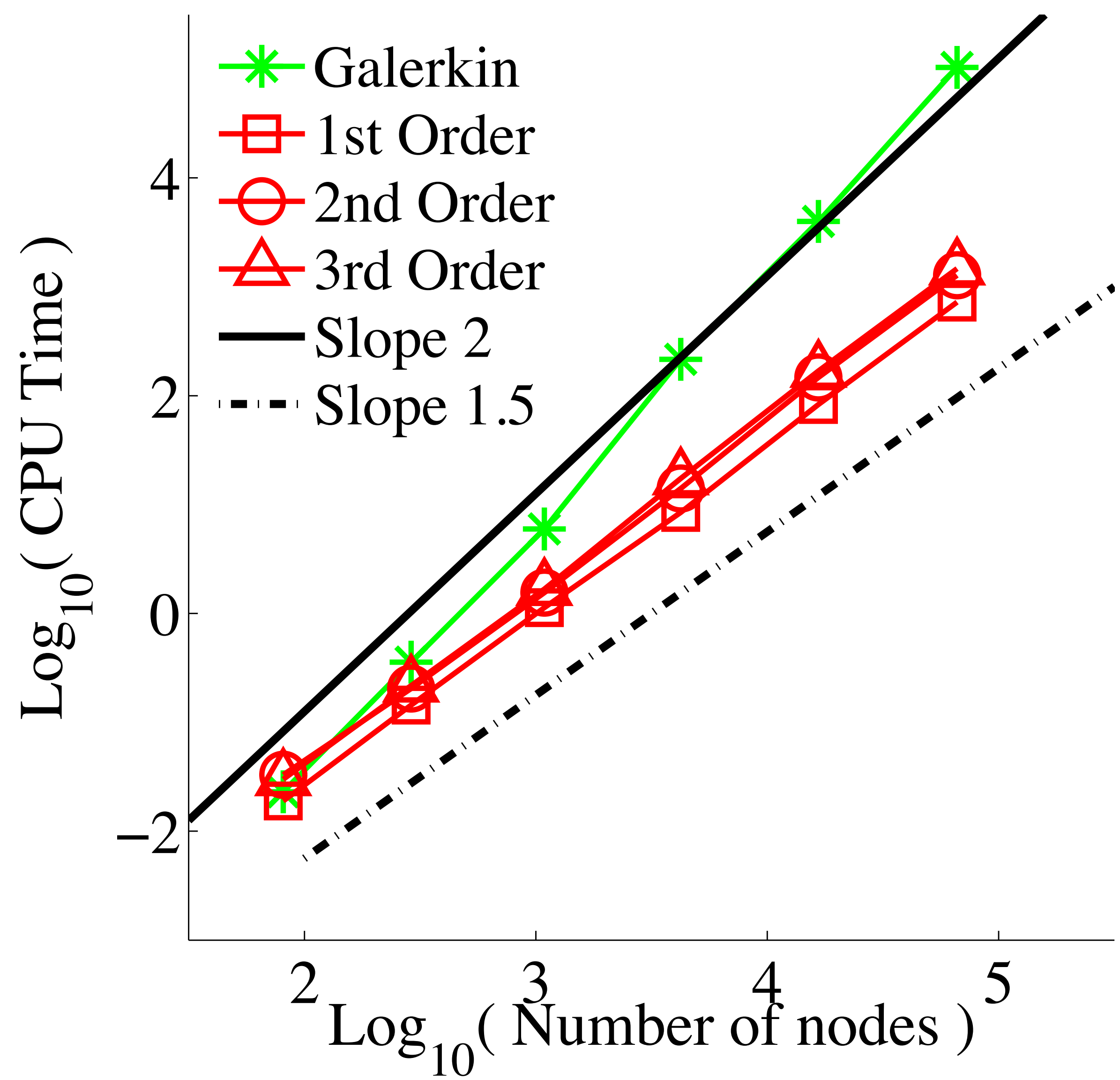
Almost the same.

Reality is that hyperbolic schemes are more economical because they converge O(1/h) faster than typical diffusion schemes.

Time to Solution

O(1/h) acceleration overwhelms the increased cost per time step.





Orders of magnitude acceleration in CPU time.

Conclusions

Diffusion and source recreated hyperbolic.

1. *Energy-stable first-order diffusion scheme*

2. *Equal order of accuracy for sol. and gradients on irregular grids.*

3. *Third-order diffusion scheme by fully hyperbolic system*

Third-order scheme is incomparably efficient and accurate.

Future Work

Uniformly third-order advection-diffusion scheme.
Implicit schemes.
Time-dependent problems.
Third-order scheme for Navier-Stokes (2nd-order scheme in AIAA2011).
New system for accurate velocity gradients (vorticity, turb source).
Hyperbolic formulation for turbulence models (robust diffusion).

Various Other Applications:

- *High-order residual-distribution schemes, dispersion eq., Incomp. NS at INRIA*
- *3rd-order active flux scheme at University of Michigan*
- *Entropy-consistent scheme at Universiti Sains Malaysia*
- *Many other potential applications: DG, SV, CESE, SUPG, etc.*

Declaration of Hyperbolicity

We hold these truths to be self-evident, that all PDEs are created equal, that they are endowed by us with certain unalienable Rights, that among these are hyperbolicity, consistent and accurate schemes and the pursuit of robustness.