Divergence Formulation of Source Term

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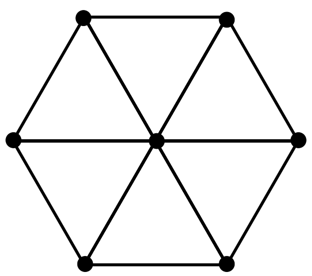
Give Up or Never Give Up

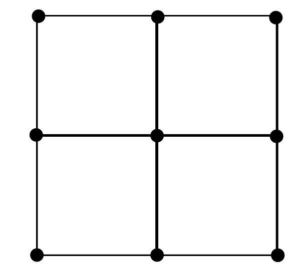
"There're times when it is good to give up."
"I agree."

I give up to get creative.

Interesting Schemes

Economical high-order schemes





Residual-distribution schemes (Roe, VKI, INRIA, etc.)

Residual-based compact schemes (Corre and Lerat, JCP2001)

Third-order edge-based finite-volume scheme (Katz and Sankaran JCP2011)

These schemes contain the target equation (or residual) in the truncation error (TE):

E.g., for linear advection, an RD scheme has the following TE,

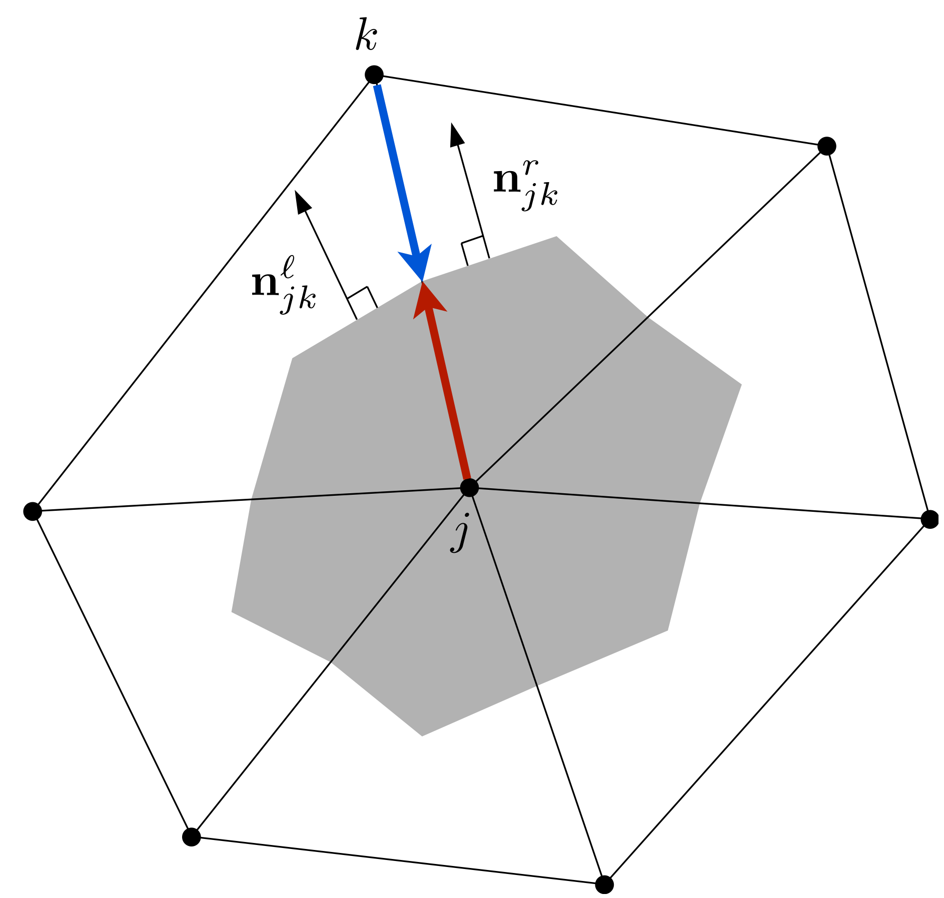
$$\mathcal{TE} = \frac{h}{2a}(a\partial_x + b\partial_y)(a\partial_x u + b\partial_y u) + O(h^2)$$

Leading term vanishes in steady state, and accuracy upgraded to second-order (Residual property).

This talk will focus on the third-order FV scheme for conservation laws with a source term.

Second-Order FV Scheme

Conservation law: $\partial_x f + \partial_y g = 0$



Edge-based finite-volume scheme:

$$0 = -\sum_{k \in \{k_j\}} \phi_{jk} A_{jk}$$

with the upwind flux at edge midpoint:

$$\phi_{jk} = \frac{1}{2}(\mathbf{F}_L + \mathbf{F}_R) \cdot \hat{\mathbf{n}}_{jk} - \frac{1}{2}|\lambda|(u_R - u_L)$$

with the left and right solution values:

$$u_L = u_j + \frac{1}{2}(\nabla u)_j \cdot \Delta \mathbf{l}_{jk}, \quad u_R = u_k - \frac{1}{2}(\nabla u)_k \cdot \Delta \mathbf{l}_{jk}$$

$$A_{jk} = |\mathbf{n}^\ell_{jk} + \mathbf{n}^r_{jk}|$$

$$\hat{\mathbf{n}}_{jk} = (\mathbf{n}^\ell_{jk} + \mathbf{n}^r_{jk})/A_{jk}$$

$$\mathbf{F} = (f, g)$$

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

$$\lambda = (\partial_u f, \partial_u g) \cdot \hat{\mathbf{n}}_{jk}$$

Second-order accurate with first-order accurate gradients.

NASA's FUN3D, Software Cradle's SC/Tetra, etc.

Third-Order FV Scheme

(Katz and Sankaran JCP2011)

1. Extrapolate the fluxes: $\phi_{jk} = \frac{1}{2}(\mathbf{F}_L + \mathbf{F}_R)\cdot\hat{\mathbf{n}}_{jk} - \frac{1}{2}|\lambda|(u_R - u_L)$

Left and right fluxes are computed by

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

2. Second-order gradients (e.g., LSQ quadratic fit)

$$(\nabla u)_j = \sum_{k\in\{k_j\}} (u_k - u_j) \begin{bmatrix} c^x_{jk} \\ c^y_{jk} \end{bmatrix} \qquad (\nabla\mathbf{F})_j = \begin{bmatrix} \frac{\partial f}{\partial u}u_x & \frac{\partial f}{\partial u}u_y \\ \frac{\partial g}{\partial u}u_x & \frac{\partial g}{\partial u}u_y \end{bmatrix}_j$$

LSQ coefficients

The resulting scheme has the truncation error on triangular(tetrahedral) grids:

$$\mathcal{TE} = (C_1\partial_{xx} + C_2\partial_{xy} + C_3\partial_{yy})(\partial_x f + \partial_y g)h^2 + O(h^3)$$

Third-order scheme on second-order stencil

Conservation Law with Source

For a conservation law with a source term:

$$\partial_x f + \partial_y g = s$$

Source term includes a time-derivative term.

We add a source term discretization to the third-order scheme:

$$0 = -\sum_{k\in\{k_j\}} \phi_{jk} A_{jk} + \int_{V_j} s\, dV$$

$$\int_{V_j} s\, dV = s_j V_j$$

Source term must be discretized to yield

$$\mathcal{TE} = (C_1 \partial_{xx} + C_2 \partial_{xy} + C_3 \partial_{yy})(\partial_x f + \partial_y g - s)h^2 + O(h^3)$$

This is critical for extending the third-order scheme to time-dependent problems.

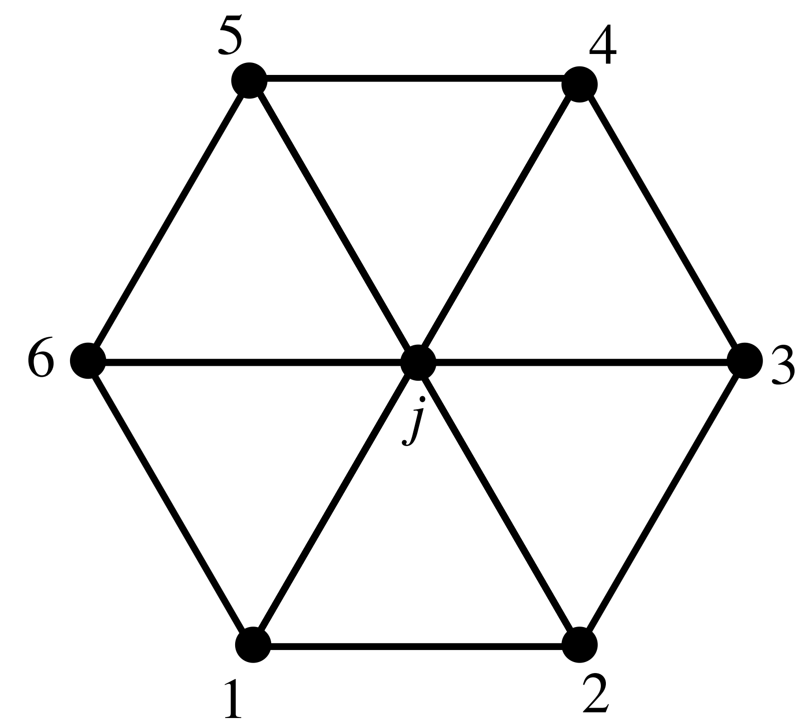
Special formulas exist for regular grids.

Formulas for Regular Grids

Equilateral-triangular stencil:

$$\int_{V_j} s\, dV = \frac{V_j}{12}(6s_j + s_1 + s_2 + s_3 + s_4 + s_5 + s_6)$$

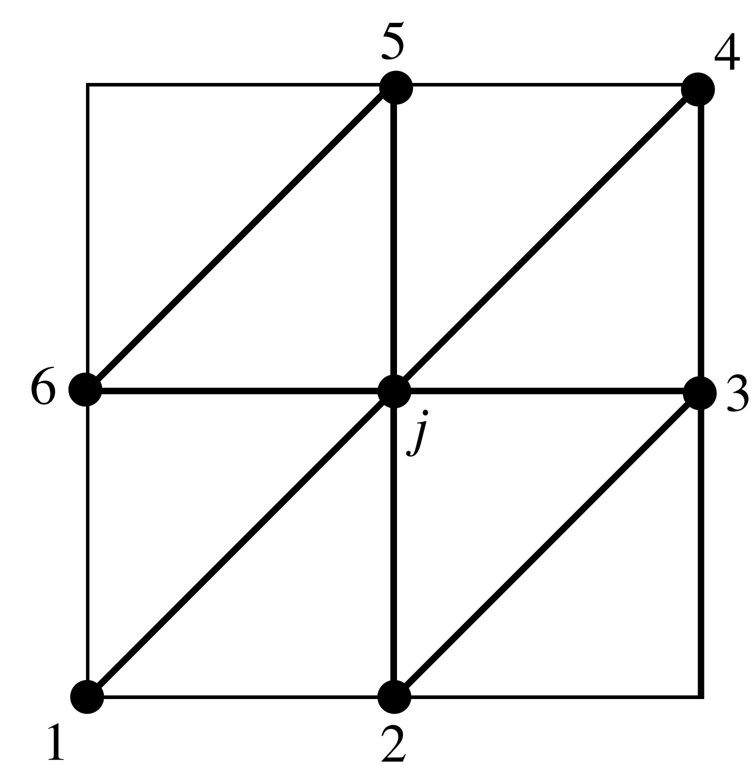
Galerkin Discretization (Katz and Sankaran JCP2011)



Right-triangular stencil:

$$\int_{V_j} s\, dV = \frac{V_j}{24}(30s_j - s_1 - s_2 - s_3 - s_4 - s_5 - s_6)$$

(Nishikawa, JCP2012)



How can I come up with such a formula for irregular grids?

I can't.

New Problem

Can we write the source term in the divergence form?

$$s \longrightarrow \partial_x f^s + \partial_y g^s$$

If possible, we can write

$$\partial_x f + \partial_y g = s$$

$$\longrightarrow \quad \partial_x f + \partial_y g = \partial_x f^s + \partial_y g^s$$

$$\longrightarrow \quad \partial_x (f - f^s) + \partial_y (g - g^s) = 0$$

Then, source term discretization will not be needed.

Nishikawa, JCP2012

Divergence Formulation of Source Term

$$s \longrightarrow \partial_x f^s + \partial_y g^s$$

where

$$f^s = \frac{1}{2}(x - x_j)s + \frac{1}{4}(x - x_j)^2 \partial_x s + \frac{1}{12}(x - x_j)^3 \partial_{xx} s$$

$$g^s = \frac{1}{2}(y - y_j)s + \frac{1}{4}(y - y_j)^2 \partial_y s + \frac{1}{12}(y - y_j)^3 \partial_{yy} s$$

(xj, yj) is a point in a computational grid.

Then, $\partial_x f + \partial_y g = s$ can be written as a single divergence form:

$$\partial_x (f - f^s) + \partial_y (g - g^s) = 0$$

Source term discretization is no longer needed.

Gradient and Hessian of the source are needed,
which can be computed by the quadratic fit.

Equivalent up to Third-Order

The divergence form,

$$\partial_x (f - f^s) + \partial_y (g - g^s) = 0$$

can be expanded as

$$\underline{\partial_x f + \partial_y g =} \; s + \frac{1}{12}(x - x_j)^3 \partial_{xxx} s + \frac{1}{12}(y - y_j)^3 \partial_{yyy} s$$

At node j, it is equivalent to the original equation.
In the neighborhood, equivalent up to third-order,

which is sufficient for third-order scheme.

One-Component Forms

The divergence form is equivalent to the following:

$$f^s = (x - x_j)s + \frac{1}{2}(x - x_j)^2 \partial_x s + \frac{1}{6}(x - x_j)^3 \partial_{xx} s$$

$$g^s = 0$$

or

$$f^s = 0$$

$$g^s = (y - y_j)s + \frac{1}{2}(y - y_j)^2 \partial_y s + \frac{1}{6}(y - y_j)^3 \partial_{yy} s$$

All are equivalent to one another up to third-order.

Nishikawa, JCP2012

Third-Order Scheme

Conservation law: $\partial_x(f - f^s) + \partial_y(g - g^s) = 0$

Edge-based finite-volume scheme:

$$0 = -\sum_{k \in \{k_j\}} (\phi_{jk} + \psi_{jk}) A_{jk}$$

with the central flux for the source flux:

$$\psi_{jk} = \frac{1}{2}(\mathbf{F}^s_L + \mathbf{F}^s_R) \cdot \hat{\mathbf{n}}_{jk} \qquad \mathbf{F}^s = (f^s, g^s)$$

with the left and right flux values:

$$\mathbf{F}^s_L = \mathbf{F}^s_j + \frac{1}{2}(\nabla \mathbf{F}^s)_j \cdot \Delta \mathbf{l}_{jk}, \quad \mathbf{F}^s_R = \mathbf{F}^s_k - \frac{1}{2}(\nabla \mathbf{F}^s)_k \cdot \Delta \mathbf{l}_{jk}$$

The resulting scheme has the truncation error:

$$\mathcal{TE} = (C_1 \partial_{xx} + C_2 \partial_{xy} + C_3 \partial_{yy})(\partial_x f + \partial_y g - s)h^2 + O(h^3)$$

Third-order achieved without source term discretization.

One-Component Case

$$f^s = (x - x_j)s + \frac{1}{2}(x - x_j)^2 \partial_x s + \frac{1}{6}(x - x_j)^3 \partial_{xx} s$$

$$g^s = 0$$

Edge-based finite-volume scheme:

$$0 = - \sum_{k \in \{k_j\}} (\phi_{jk} + \psi_{jk}) A_{jk} \qquad 0 = - \sum_{k \in \{k_j\}} \phi_{jk} A_{jk} + \int_{V_j} s \, dV$$

with the central flux for the source flux:

$$\psi_{jk} = \frac{1}{2}(f_L^s + f_R^s, 0) \cdot \hat{\mathbf{n}}_{jk}$$

with the left and right flux values:

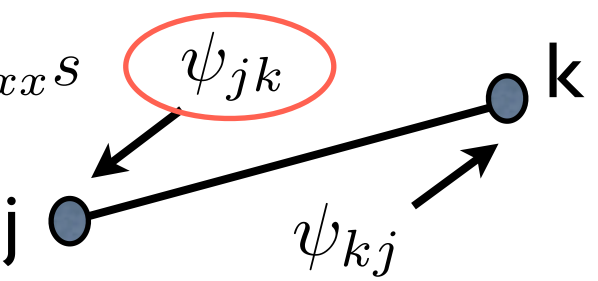
$$f_L^s = f_j^s + \frac{1}{2}(\nabla f^s)_j \cdot \Delta \mathbf{l}_{jk}, \quad f_R^s = f_k^s - \frac{1}{2}(\nabla f^s)_k \cdot \Delta \mathbf{l}_{jk}$$

Source discretization replaced by a scalar central scheme.

Some details not given in Nishikawa, JCP2012

Source Flux and Flux Gradients

Source flux: $f^s = (x - x_j)s + \frac{1}{2}(x - x_j)^2 \partial_x s + \frac{1}{6}(x - x_j)^3 \partial_{xx} s$



1. Compute the source flux at nodes:

$$f_j^s = 0, \quad f_k^s = (x_k - x_j)s_k + \frac{1}{2}(x_k - x_j)^2 \partial_x s_k + \frac{1}{6}(x_k - x_j)^3 \partial_{xx} s_k$$

2. Compute the gradient of the source flux:

Ignored for third-order

$$(\nabla f)_j = \begin{bmatrix} s_j \\ 0 \end{bmatrix} \quad (\nabla f)_k = \begin{bmatrix} s_k + \frac{1}{6}(x_k - x_j)^3 \partial_{xxx} s_k \\ (x_k - x_j)\partial_y s_k + \frac{1}{2}(x_k - x_j)^2 \partial_{xy} s_k + \frac{1}{6}(x_k - x_j)^3 \partial_{xxy} s_k \end{bmatrix}$$

Ignored for third-order

3. Compute the left and right fluxes:

$$f_L^s = f_j^s + \frac{1}{2}(\nabla f^s)_j \cdot \Delta \mathbf{l}_{jk}, \quad f_R^s = f_k^s - \frac{1}{2}(\nabla f^s)_k \cdot \Delta \mathbf{l}_{jk}$$

4. Compute the central flux for node j: $\psi_{jk} = \frac{1}{2}(f_L^s + f_R^s, 0) \cdot \hat{\mathbf{n}}_{jk}$

The other flux needs to be computed separately because $\psi_{jk} \neq -\psi_{kj}$.

Source flux discretization is not conservative (of course).

Exact Divergence Form

If the source term is simple enough, e.g.,

$$\partial_x f + \partial_y g = \cos(x - y)$$

it can be written exactly as

$$\partial_x f + \partial_y g = \partial_x f^s + \partial_y g^s$$

$$f^s = \sin(x - y), \quad g^s = 0$$ (The choice is not unique.)

Therefore, again, source term discretization is not needed.

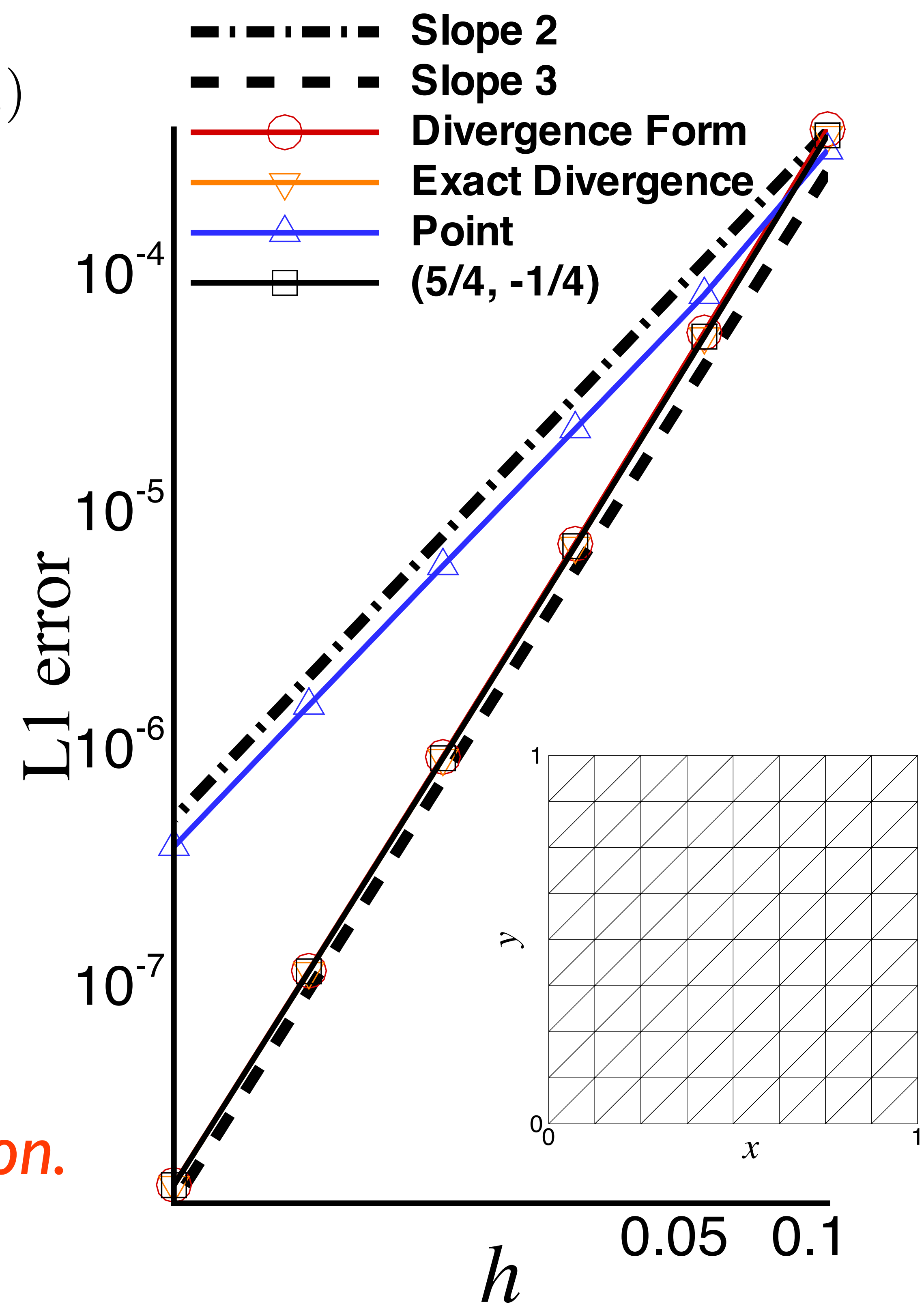
1. *Second derivatives are not needed.*
2. *Gradient of the source term is needed.*
   (It can be computed analytically or by a quadratic fit.)
3. *This is not possible for time-derivative terms (only discrete values).*

Burgers Equation: *Regular Grids*

$$\partial_x(u^2/2) + \partial_y u = \cos(x-y)(\sin(x-y)-1)$$

Exact solution: $u(x,y) = \sin(x-y)$

- n x n grids: n = 9, 17, 33, 65, 129, 257.
- Dirichlet boundary condition.
- 6 neighbors for quadratic fit.
- Time-stepping by RK2 to steady state.
- (5/4, -1/4) indicates the special formula.



Second-order with the point discretization.

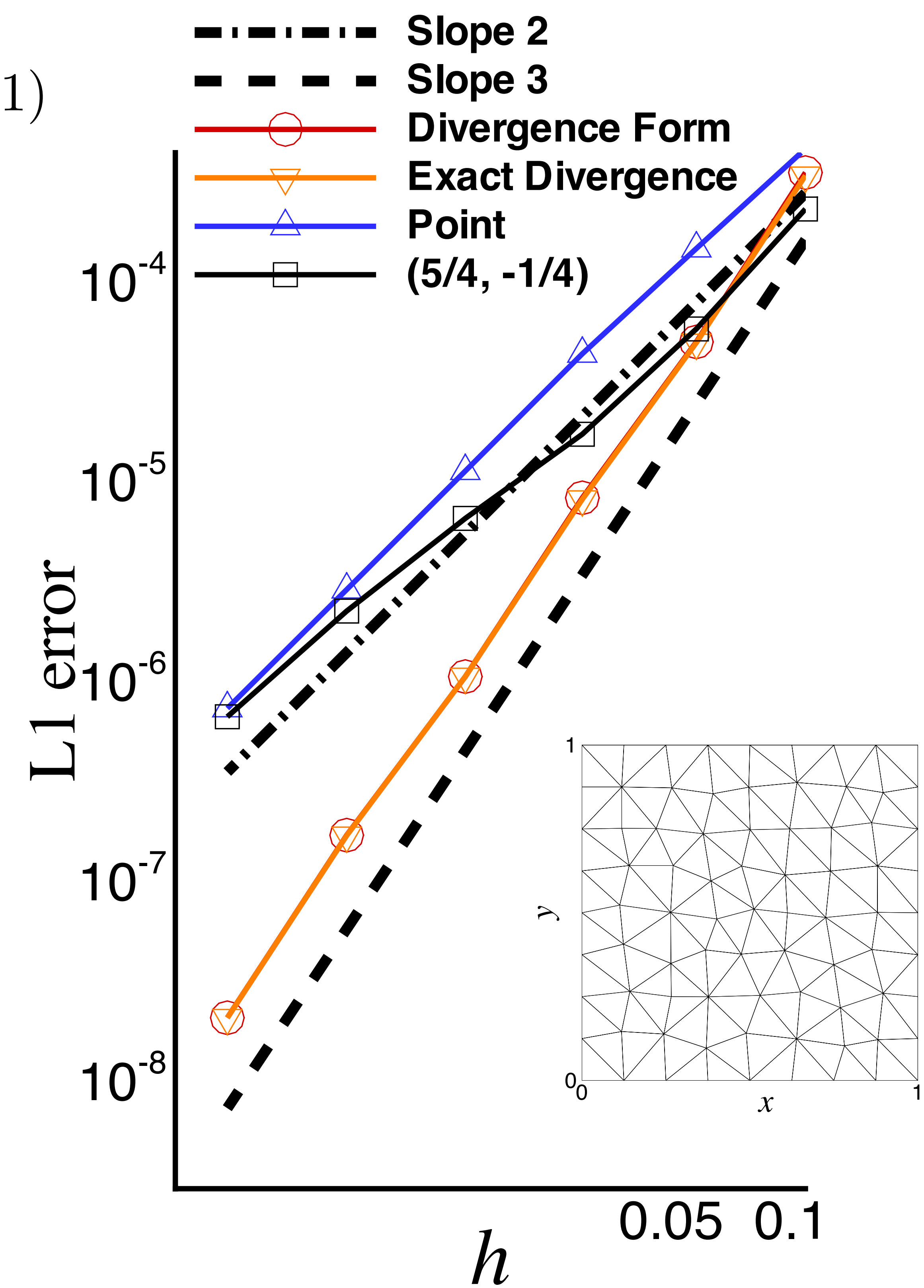
Burgers Equation: *Irregular Grids*

$$\partial_x(u^2/2) + \partial_y u = \cos(x-y)(\sin(x-y)-1)$$

Exact solution: $u(x,y) = \sin(x-y)$

- 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)
- Time-stepping by RK2 to steady state.
- (5/4, -1/4) indicates the special formula.

Only the divergence formulation achieved third-order accuracy.



Conclusion

Third-order finite-volume scheme made simple
for source term by the divergence formulation.

Future work:

Relation with the formula of Katz (Katz 2012, unpublished); looks similar.
Application to unsteady computation (time derivative as a source).
Application to other discretization methods.
Application to other types of source terms (involving the solution). → *Hyperbolic*

which I might have never been able to even think about
if I had not given up.