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Numerical Solution of Initial Boundary Value Problems

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Multiple dimensions: FDM, FVM, DG

• All the methods discussed below are of SBP-SAT type.

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- Stability and conservation should be guaranteed.
- Overlapping/sliding methods not included.

FDM on SBP-SAT form

Would Interface Conditions SBP SAT-MB Take face condition must be concernative and stable. Map to 27 SE= const. sy=const. (Weale boundary and how Myit right 10/1 $(1+r(An)_{y} + (Bn)_{y} = 0) = 0$ $(1+r(An)_{y} + (Bn)_{y} = 0)$ ×.i,N

Kronecker products

For arbitrary matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$, the Kronecker product is defined as

$$A \otimes B = \begin{bmatrix} a_{1,1}B & \dots & a_{1,m}B \\ \vdots & \ddots & \vdots \\ a_{n,1}B & \dots & a_{m,n}B \end{bmatrix}.$$
 (1)

The Kronecker product is bilinear, associative and obeys

$$(A \otimes B)(C \otimes D) = (AC \otimes BD)$$
(2)

if the usual matrix products are defined. For inversion and transposing we have

$$(A \otimes B)^{-1,T} = A^{-1,T} \otimes B^{-1,T}$$
(3)

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if the usual matrix inverse is defined.

Organisation

$$\frac{\partial F}{\partial x} \approx (P_x^{-1}Q_x \otimes I_y)\vec{F} = (P_x^{-1}Q_x \otimes I_y \otimes I_4)\vec{F} = (P_x^{-1}Q_x \otimes I_y \otimes A)\vec{u}$$
$$\frac{\partial G}{\partial y} \approx (I_x \otimes P_y^{-1}Q_y)\vec{G} = (I_x \otimes P_y^{-1}Q_y \otimes I_4)\vec{G} = (I_x \otimes P_y^{-1}Q_y \otimes B)\vec{u}$$





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The semi-discrete schemes

Focus only at the interface:

$$u_t + (P_x^{-1}Q_x \otimes I_y)\vec{F} + (I_x \otimes P_y^{-1}Q_y)\vec{G} = (P_x^{-1} \otimes I_y)\Sigma_L(u-v)$$
$$v_t + (P_x^{-1}Q_x \otimes I_y)\vec{F} + (I_x \otimes P_y^{-1}Q_y)\vec{G} = (P_x^{-1} \otimes I_y)\Sigma_R(v-u)$$

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Determine Σ_L , Σ_R such that the coupling is stable and conservative.

<u>Conservation</u> $\phi = \phi(x, y, t) = \text{smooth}, \phi(\pm \infty, \pm \infty, t) = 0.$ $\phi^T(P_x \otimes P_y)u_t + \phi^T(Q_x \otimes P_y)F + \phi^T(P_x \otimes Q_y)G = \phi^T(I_x \otimes P_y)\Sigma_L(u - v)$

SBP:
$$Q_x \rightarrow -Q_x^T + B_x$$

 $Q_y \rightarrow -Q_y^T + B_y$

$$\phi^{T}(P_{x} \otimes P_{y})u_{t} - \phi^{T}(Q_{x}^{T} \otimes P_{y})F - \phi^{T}(P_{x} \otimes Q_{y}^{T})G + \phi^{T}(B_{x} \otimes P_{y})F + \phi^{T}(P_{x} \otimes B_{y})G = \phi^{T}(I_{x} \otimes P_{y})\Sigma_{L}(u - v)$$

 $\underbrace{Note}_{\phi^{T}(Q_{x}^{T} \otimes P_{y})F = \phi^{T}(Q_{x}^{T} \otimes I_{y})(I_{x} \otimes P_{y})F =}_{\phi^{T}(Q_{x}^{T} \otimes I_{y})((P_{x}^{-1})^{T} \otimes I_{y})}\underbrace{(P_{x} \otimes I_{y})(I_{x} \otimes P_{y})}_{\phi^{T}_{x}}F = \phi^{T}_{x}(P_{x} \otimes P_{y})F$

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Same procedure as in one dimension, all derivatives flipped \Rightarrow

$$\phi^T (P_x \otimes P_y) u_t - \phi_x^T (P_x \otimes P_y) F - \phi_y^T (P_x \otimes P_y) G =$$

Boundary terms at i = 0 for all gridpoint j = 0, M.



From the other equation we get the corresponding terms

$$IT_R = \phi_0^T (P_y^R \otimes A) v_0 + \phi_0^T (P_y^R \otimes \tilde{\Sigma_R}) (v_0 - u_N).$$

Conservation at interface requires $IT_L + IT_R = 0$, hence

$$IT_L + IT_R = (\phi_0 = \phi_N = \phi_i, \ P_y^L = P_y^R = P_y) = \phi_i^T (P_y \otimes (-A + \tilde{\Sigma_L} - \tilde{\Sigma_R})(u_N - v_0)) = 0$$

lead to conservation.

 $\therefore \quad \tilde{\Sigma_L} = \tilde{\Sigma_R} + A$ is the conservation condition.

Note similarity with 1D $\sigma_L = \sigma_R + a$

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The same technique, multiplying from left with $u^T(P_x \otimes P_y) \Rightarrow$

$$\frac{d}{dt}(u^{T}(P_{x}^{L}\otimes P_{y}^{L})u+v^{T}(P_{x}^{R}\otimes P_{y}^{R})v) = \\ \begin{bmatrix} u_{N} \\ v_{0} \end{bmatrix}^{T} \underbrace{\begin{bmatrix} P_{y}\otimes(-A+2\Sigma_{L}) & P_{y}\otimes(-\Sigma_{L}-\Sigma_{R}) \\ P_{y}\otimes(-\Sigma_{R}-\Sigma_{L}) & P_{y}\otimes(A+2\Sigma_{R}) \end{bmatrix}}_{\tilde{A}} \begin{bmatrix} u_{N} \\ v_{0} \end{bmatrix}$$

Recall $A \otimes B = a_{ij}B$, Unfortunately, this is not the form of \tilde{A} .

However there exists ψ such that $P_y \otimes A_{ij} = \psi^T (A_{ij} \otimes P_y) \psi$. "even permutation similar." \Rightarrow

$$\begin{bmatrix} u_{N} \\ v_{0} \end{bmatrix}^{T} \begin{bmatrix} \psi^{T}(A_{11} \otimes P_{y})\psi & \psi^{T}(A_{12} \otimes P_{y})\psi \\ \psi^{T}(A_{12} \otimes P_{y})\psi & \psi^{T}(A_{22} \otimes P_{y})\psi \end{bmatrix} \begin{bmatrix} u_{N} \\ v_{0} \end{bmatrix}$$
$$\begin{bmatrix} \psi u_{N} \\ \psi v_{0} \end{bmatrix}^{T} \begin{bmatrix} A_{11} \otimes P_{y} & A_{12} \otimes P_{y} \\ A_{12} \otimes P_{y} & A_{22} \otimes P_{y} \end{bmatrix} \begin{bmatrix} \psi u_{N} \\ \psi v_{0} \end{bmatrix}$$
$$\underbrace{\begin{bmatrix} A_{11} & A_{12} \\ A_{12} & A_{22} \end{bmatrix}}_{\tilde{A}} \otimes P_{y}$$

For stability we need $\tilde{\tilde{A}} \leq 0$. The conservation condition in $\tilde{\tilde{A}} \Rightarrow$

$$\begin{bmatrix} -A + 2\Sigma_L & -2\Sigma_L + A \\ -2\Sigma_L + A & -A + 2\Sigma_L \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & -1 \\ -1 & 1 \\ \\ \lambda = 0, 2 \end{bmatrix}}_{\lambda = 0, 2} \otimes \underbrace{\begin{bmatrix} -A + 2\Sigma_L \end{bmatrix}}_{\leq 0}$$

∴ Stability if conservation condition holds and $-A + 2\Sigma_L \leq 0$.

We need $2\Sigma_L - A \le 0$. However $A = X\Lambda X^T = X(\Lambda^+ + \Lambda^-)X^T$. Let $\Sigma_L = X\tilde{\Sigma}_L X^T \Rightarrow$ $2\Sigma_L - A = X^T (2\bar{\Sigma}_L - \Lambda^+ - \Lambda^-)X = -X\Lambda^+ X^T + X(2\tilde{\Sigma}_L - \Lambda^-)X^T$ 1st choice $\Sigma_L = \frac{\Lambda^-}{2}$ damping by $-A^+$ 2nd choice $\Sigma_L = \Lambda^-$ damping by $A^- - A^+$

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Summary of the SBP-SAT-MB technique

- It is a conservative and stable method.
- Nodes on interface must coincide.
- The integration operators (norms) must be the same on both sides of interface.
- If the norms are different, interpolation operators must be used.
- If the nodes do not coincide, interpolation operators must be used.
- The stability and conservation conditions are similar to the one-dimensional ones.

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Node centered unstructured finite volume methods



SBP operators

Boundaries





 \therefore $Q_x + Q_x^T = \Delta Y$, elements of $\Delta Y \neq 0$ only at boundary points.

 $\therefore Q_y^T + Q_y^T = -\Delta X$, elements of $\Delta X \neq 0$ only at boundaries.

... The UFVM yields SBP operators.

Boundary procedures

What about boundary bonditions and SAT?

$$u_t + Au_x + Bu_y = 0, \ \vec{x} \in \Omega$$
$$Lu = g, \ \vec{x} \in \partial \Omega$$
$$u(\vec{x}, 0) = f, \ \vec{x} \in \Omega$$

Let *A*, *B* be symmetric and consider the energy.

$$\int_{\Omega} uu_t dx dy + \int_{\Omega} u^T (Au)_x + u^T (Bu)_y dx dy = 0 \implies \frac{1}{2} ||u||_t^2 + \frac{1}{2} \int_{\Omega} (u^T Au)_x + (u^T Bu)_y dx dy = 0 \implies$$

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Boundary procedures

$$||u||_t^2 + \oint_{\partial\Omega} u^T A u dy - u^T B u dx = 0 \Rightarrow$$

$$\|u\|_{t}^{2} + \oint_{\partial\Omega} u^{T} \underbrace{((A, B) \cdot \vec{n})}_{\tilde{A} = symmetric} uds = 0, \quad \tilde{A} = X\Lambda_{A}X^{T}, \quad \Lambda_{A} = \Lambda_{A}^{+} + \Lambda_{A}^{-} \Rightarrow$$

$$||u||_t^2 + \oint_{\partial\Omega} u^T X(\Lambda_A^+ + \Lambda_A^-) X^T u \, ds = 0, \quad \Lambda_A^- \text{ dangerous.}$$

Use the characteristic boundary condition $(X^T u)^- = (X^T \overline{u})^- \Rightarrow$

$$\frac{d}{dt}||u||^2 + \oint_{\partial\Omega} u^T A^+ u + \bar{u}^T A^- \bar{u} ds = 0.$$
(6)

 \therefore A well-posed problem.

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Conservation

Is the scheme $Pu_t + (Q_x \otimes A)u + (Q_y \otimes B)u = 0$ conservative ?

$$\phi^{T}Pu_{t} + \phi^{T}(Q_{x} \otimes A)u + \phi^{T}(Q_{y} \otimes B)u = 0$$

$$Q_{x} = -Q_{x}^{T} + \Delta Y, \quad Q_{y} = -Q_{y}^{T} - \Delta X \Rightarrow$$

$$\phi^{T}Pu_{t} - \phi^{T}(Q_{x}^{T} \otimes A)u - \phi^{T}(Q_{y}^{T} \otimes B)$$

$$+\phi^{T}(\Delta Y \otimes A)u + \phi^{T}(-\Delta X \otimes B)u = 0$$

$$\phi^{T}Pu_{t} - \left[(Q_{x} \otimes I)\phi\right]^{T}[I \otimes A]u - \left[(Q_{y} \otimes I)\phi\right]^{T}[I \otimes B]u$$

$$+ \sum_{i} \phi_{i}((A, B) \cdot \vec{n_{i}})u_{i}ds_{i}$$

$$BT$$

.: No remaining interiour terms: Conservative!

Stability of UFVM

$$(P \otimes I)u_t + (Q_x \otimes A)u + (Q_y \otimes B)u = (E_B^T \otimes I)\underbrace{\Sigma(u - G)}_H$$

 E_B picks out boundary points. Non-zero on the boundary only. $u^T(P \otimes I)u_t + u^T(Q_x \otimes A) + u^T(Q_y \otimes B)u = u^T(E_B^T \otimes I)H =$

$$= ((E_B \otimes I)u)^T H = u_B^T H = \sum_{i \in B} u_{Bi}^T H_i = \sum u_i^T \Sigma_i (u - \bar{u})_i$$

$$(||u||_{P\otimes I}^2)_t + u^T (\Delta Y \otimes A)u + u^T (-\Delta X \otimes B)u = 2u_B^T H.$$

$$(||u||_{P\otimes I}^{2})_{t} = \sum_{i} -u_{i}^{T}((A, B) \cdot \vec{n_{i}})u_{i}ds_{i} + 2u_{i}^{T}\Sigma_{i}(u_{i} - \bar{u}_{i})$$
$$= \sum_{i} \left(-u_{i}^{T}\tilde{A}_{i}u_{i} + 2u_{i}^{T}\tilde{\Sigma}_{i}(u_{i} - \bar{u}_{i})\right)ds_{i}$$

Energy estimate

$$\tilde{A}_i = \tilde{A}_i^+ + \tilde{A}_i^- \Rightarrow \sum_i \left(-u_i^T A_i^+ u_i - u_i^T (A_i^- - 2\tilde{\Sigma}_i) u_i - 2u_i \tilde{\Sigma}_i \bar{u}_i \right) ds_i.$$

Let $\Sigma_i = +A_i^- \Rightarrow$

$$\frac{d}{dt}(||u||_{P\otimes I}^{2}) + \sum_{i\in B} u_{i}^{T}A^{+}u_{i} + \bar{u}_{i}^{T}A^{-}\bar{u}_{i}ds_{i} = \underbrace{\sum_{i\in B} (u-\bar{u}_{i})^{T}A_{i}^{-}(u-\bar{u}_{i})ds_{i}}_{\leq 0}.$$

: An estimate in terms of data !

: UFVM both conservative and stable.

: Warning ! Could be suprisingly inaccurate with O(1) errors.

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SBP-SAT-MB + UFVM = Hybrid



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Discontinuous Galerkin (DG)



 $u_t + (Au)_x + (Bu)_y = 0$, F = Au, G = Bu, u = solution vector $A = A^T$, $B = B^T =$ constant matrices

1. Multiply with smooth function $\alpha = \alpha(x, y, t)$.

$$\int_{\Omega_i} \alpha u_t \, dx \, dy + \int_{\Omega_i} \alpha F_x + \alpha G_y \, dx \, dy = 0$$

Derivation of penalty term

2) Integrate-by-parts

$$\int_{\Omega_{i}} \alpha u_{t} \, dx \, dy + \int_{\Omega_{i}} (\alpha F)_{x} + (\alpha G)_{y} \, dx \, dy - \int_{\Omega_{i}} \nabla \alpha \cdot \vec{F} \, dx \, dy = 0$$

where $\vec{F} = (F, G)$. Green-Gauss \Rightarrow
$$\int_{\Omega_{i}} \alpha u_{t} d\Omega - \int_{\Omega_{i}} \nabla \alpha \cdot \vec{F} d\Omega + \oint_{\partial \Omega_{i}} \alpha F dy - \alpha G dx = 0$$
$$\int_{\Omega_{i}} \alpha u_{t} d\Omega - \int_{\Omega_{i}} \nabla \alpha \cdot \vec{F} d\Omega + \oint_{\partial \Omega_{i}} \alpha \vec{F} \cdot \vec{n} ds = 0$$

3) Change $F \rightarrow \hat{F}$ = numerical Flux= what you want it do be.

Derivation of penalty term

$$\int_{\Omega_i} \alpha u_t - \nabla \alpha \cdot F d\Omega + \oint_{\partial \Omega_i} \alpha \hat{F} \cdot \vec{n} ds = 0$$
(7)

Integrate back \Rightarrow

$$\int_{\Omega_i} \alpha u_t + \alpha \nabla \cdot F d\Omega + \underbrace{\oint_{\partial \Omega_i} \alpha(\hat{F} - F) \cdot \vec{u} ds}_{\text{penalty term}} = 0$$
(8)

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A penalty term just as in the SBP-SAT technique.

Conservation

Look at two nearby elements. Let $\alpha = \phi$.

$$\int_{\partial\Omega_i}\phi_i\hat{F}_i\cdot\vec{n}_ids+\int_{\partial\Omega_{i+1}}\phi_{i+1}\hat{F}_{i+1}\cdot\vec{n}_{i+1}ds=$$

$$= (\vec{n}_{i+1} = -\vec{n}_i, \phi_{i+1} = \phi_i) = \int_{\partial \Omega_i} \phi_i \hat{F}_i \cdot n_i + \phi_{i+1} \hat{F}_{i+1} (-\vec{n}_i) ds$$

$$= \int_{\partial \Omega_i} \phi_i(\vec{\hat{F}}_i - \vec{\hat{F}}_{i+1}) \cdot \vec{n}_i ds.$$

 \therefore No terms at the interface if $(\vec{F}_i - \vec{F}_{i+1}) \cdot \vec{n}_i = 0$.

... DG is a conservative if numerical fluxes on adjacent elements are the same.

Let $\alpha = u \Rightarrow$ $\int_{\Omega} u u_t d\Omega + \int_{\Omega} u^T (A u)_x + u^T (B u)_y d\Omega$ $+ \int_{-\infty}^{\infty} u^{T}(\hat{F} - F) \cdot \vec{n} ds = 0$ $\frac{1}{2} \|u\|_t^2 + \frac{1}{2} \int_{\partial \Omega_t} \underbrace{u^T A u dy - u^T B u}_{-} dx + \oint_{\partial \Omega_t} u^T (\hat{F} - F) \cdot \vec{n} ds = 0$ u^TF·nds $||u||_t^2 + 2 \oint_{i=0}^{\infty} u^T (\hat{F} - \frac{1}{2}F) \cdot \vec{n} ds = 0.$

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The other side \Rightarrow

$$(||u||_{i}^{2} + ||u||_{i+1}^{2})_{t} + 2 \oint_{\partial \Omega_{i}} u_{i}^{T} (\hat{F}_{i}^{T} - \frac{1}{2}F_{i}) \cdot \vec{n}_{i} ds + 2 \oint_{\partial \Omega_{i+1}} u_{i+1}^{T} (\hat{F}_{i+1}^{T} - \frac{1}{2}F_{i+1}) \cdot \vec{n}_{i+1} ds = 0$$

$$\hat{F}_i \cdot \vec{n}_i = C_0 \{F\}_i + C_1 [F]_i; \{F\}_i = (A, B) \cdot \vec{n}_i \left(\frac{u_i + u_{i+1}}{2}\right)$$

 $\hat{F}_{i+1} \cdot \vec{n}_i = C_2 \{F\}_i + C_3 [F]_i; \ [F]_i = (A, B) \cdot \vec{n}_i (u_i - u_{i+1})$

Conservation \Rightarrow $(C_0 - C_2) \{F\}_i + (C_1 - C_3) [F]_i = 0$

 $\Rightarrow \underline{C_2 = C_0, C_3 = C_1}$

$$BT = \oint u_i^T (C_0 \tilde{A} \left(\frac{u_i + u_{i+1}}{2}\right) + C_1 \tilde{A} (u_i - u_{i+1}) - \frac{1}{2} \tilde{A} u_i)$$

- $u_{i+1}^T \left(C_0 \tilde{A} \frac{u_i + u_{i+1}}{2} + C_1 \tilde{A} (u_i - u_{i+1}) - \frac{1}{2} \tilde{A} u_{i+1}\right) ds =$
= $\oint u_i^T (\frac{1}{2} (C_0 - I) + C_1) \tilde{A} u_i + u_i^T (\frac{C_0}{2} - C_1) u_{i+1}$
- $u_{i+1}^T (\frac{1}{2} (C_0 - I) - C_1) \tilde{A} u_i - u_{i+1}^T (\frac{C_0}{2} - C_1) u_i ds$

Put on matrixform, to be able to see what is going on.

$$BT = \oint \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix}^T \begin{bmatrix} (\frac{1}{2}(C_0 - I) + C_1)\tilde{A} & (\frac{C_0}{2} - C_1)\tilde{A} \\ -(\frac{C_0}{2} + C_1)\tilde{A} & (-\frac{1}{2}(C_0 - I) + C_1)\tilde{A} \end{bmatrix} \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix} ds = \\ = \oint \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix}^T \begin{bmatrix} (C_1 + \frac{C_0 - I}{2})\tilde{A} & -C_1\tilde{A} \\ -C_1\tilde{A} & (C_1 - \frac{C_0 - I}{2})\tilde{A} \end{bmatrix} \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix} ds.$$

Choose
$$C_0 = I \Rightarrow BT = \oint \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix}^T \underbrace{\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}}_{\lambda=0,+1} \otimes C_1 \tilde{A} \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix} ds$$

Need to choose C_1 such that $C_1 \tilde{A} \ge 0$.

$$\tilde{A} = X\Lambda X^T \quad C_1 = X\Sigma X^T \Rightarrow C_1 \tilde{A} = X\Sigma\Lambda X^T = X^T \Sigma (\Lambda^+ + \Lambda^-) X$$

Choose Σ such that: $\Sigma \Lambda^+ = \Lambda^+$, $\Sigma \Lambda^- = \delta |\Lambda^-| \Rightarrow$

$$C\tilde{A} = X(\Lambda^+ + \delta | \Lambda^- |) X^T = \begin{cases} A^+, \delta = 0\\ |A|, \delta = 1 \end{cases}$$

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With the above choices we find

$$\therefore BT = \oint \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix}^T \begin{bmatrix} |A| & -|A| \\ -|A| & |A| \end{bmatrix} \begin{bmatrix} u_i \\ u_{i+1} \end{bmatrix} ds = \oint (u_i - u_{i+1})^T |A| (u_i - u_{i+1}) ds \Rightarrow$$

and hence

$$\frac{d}{dt}(||u||_{i}^{2} + ||u||_{i+1}^{2}) = -\oint \underbrace{[u]|A|[u]}_{jumps} ds$$

: A stable scheme.

: Also expensive, interfaces everywhere, needed for high accuray.

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Summary of multi-dimensional schemes

- SBP-SAT-MB: Highly efficient. Requires non-nasty geometry to be optimal.
- UFVM: Can handle complex geometry, low accuracy, slow.
- DG: Very stable and accurate but expensive for high order and multiple dimensions.
- Hybrid: Combines SBP-SAT-MB + UFVM or dG. Maybe optimal by combining the best properties.
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End of Lecture 3

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