A Sparse Grid Discontinuous Galerkin Methods for High-dimensional Transport Equations

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Joint work with Wei Guo (Texas Tech)
1 Introduction

2 Numerical scheme
   - Multiresolution analysis and multiwavelets
   - DG approximation space in multi-dimensions
   - DG method on sparse grids
   - Adaptive sparse grid DG

3 Numerical tests

4 Applications in kinetic simulations

5 Conclusions
Sparse grid methods

*Breaking the curse of dimensionality – Sparse Grid & Related Techniques*

- Inspired by sparse grid quadrature Smolyak (63), introduced by Zenger (91), developed by Griebel (91,98,05...), widely used for uncertainty quantification under the collocation framework Xiu, Hesthaven (05...).

- When solving high-dimensional PDEs, sparse grid method has been incorporated in
  - Finite difference methods: Griebel (98); Griebel, Zumbusch (99).
  - Finite volume methods: Hemker (95);
  - Finite element methods: Bungartz, Griebel (04); Schwab, Suli, Todor (08);
  - Spectral methods: Griebel (07); Gradinaru (07); Shen, Wang (10); Shen, Yu (10, 12).
Hierarchical decomposition of piecewise polynomial spaces in one dimension

Consider \( \Omega = [0, 1] \) and define \( n \)-th level grid

\[
\Omega_n = \{ I^n_j = (2^{-n}j, 2^{-n}(j + 1)) \mid j = 0, \ldots, 2^n - 1 \}
\]
Hierarchical decomposition of piecewise polynomial spaces in one dimension

Conventional approximation space on the $n$-th level grid $\Omega_n$

$$V_n^k = \{ v : v \in P^k(I_j), \forall j = 0, \ldots, 2^n - 1 \}$$

$$\dim(V_n^k) = 2^n(k + 1)$$

Nested structure

$$V_0^k \subset V_1^k \subset V_2^k \subset V_3^k \subset \cdots$$

$W_n^k$: orthogonal complement of $V_{n-1}^k$ in $V_n^k$, for $n > 1$, represents the finer level details when the mesh is refined, satisfying

$$V_{n-1}^k \oplus W_n^k = V_n^k$$

$$W_n^k \perp V_{n-1}^k$$

Let $W_0^k := V_0^k$, then

$$V_N^k = \bigoplus_{0 \leq n \leq N} W_n^k$$

$$\dim(W_n^k) = \left\lceil 2^{n-1} \right\rceil (k + 1)$$
Background for multiwavelet in DG context

- Haar wavelet **Haar** (1910).
- Multiwavelet trouble cell indicator **Vuik, Ryan** (2014)...

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**Sparse grid DG**

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Hierarchical orthonormal bases

Bases in $W^k_0$: scaled orthonormal Legendre polynomials.

Bases in $W^k_1$:

$$h_i(x) = 2^{1/2} f_i(2x - 1), \quad i = 1, \ldots, k + 1$$

The orthonormal, vanishing-moment functions $\{f_i(x)\}_k$ (Alpert 93), which are supported on $(-1, 1)$ and depend on $k$, will be defined later.

Bases in $W^k_n$, $n \geq 1$

$$v_{i,n}^j(x) = 2^{(n-1)/2} h_i(2^{n-1}x - j), \quad i = 1, \ldots, k + 1, \quad j = 0, \ldots, 2^{n-1} - 1$$

Orthonormality of multiwavelet bases across different hierarchical levels

$$\int_{0}^{1} v_{i,n}^j(x) v_{i',n'}^{j'}(x) \, dx = \delta_{ii'} \delta_{nn'} \delta_{jj'}$$
Bases on different levels for $k = 0$

$\Omega_0$

$\Omega_1$

$\Omega_2$
Bases on different levels for $k = 1$
Approximation space in multi-dimensions

Consider 2D case, \( x = (x_1, x_2) \in \Omega = [0, 1]^2 \) and multi-index \( l = (l_1, l_2) \in \mathbb{N}_0^2 \)

The standard rectangular grid \( \Omega_l \) with mesh size

\[
h_l := (2^{-l_1}, 2^{-l_2})
\]

\[
h := \min\{2^{-l_1}, 2^{-l_2}\}
\]

For each \( l_l^j = \{(x_1, x_2) : x_i \in (2^{-l_1}j_i, 2^{-l_1}(j_i + 1)]\} \), the traditional tensor-product polynomial space is

\[
\mathcal{V}_l^k = \{v : v(x) \in P^k(l_l^j), \ 0 \leq j \leq 2^l - 1\}
\]

\( P^k \) denotes polynomial of degree at most \( k \) in each dimension.
Approximation space in multi-dimensions

Consider 2D case, \( x = (x_1, x_2) \in \Omega = [0, 1]^2 \) and multi-index \( l = (l_1, l_2) \in \mathbb{N}_0^2 \)

The standard rectangular grid \( \Omega_l \) with mesh size

\[
h_l := (2^{-l_1}, 2^{-l_2})
\]
\[
h := \min\{2^{-l_1}, 2^{-l_2}\}
\]

For each \( l^i_j \{ (x_1, x_2) : x_i \in (2^{-l_j}j_i, 2^{-l_j}(j_i + 1)] \} \), the traditional tensor-product polynomial space is

\[
V^k_l = \{v : v(x) \in P^k(l^i_j), \ 0 \leq j \leq 2^l - 1\}
\]

\( P^k \) denotes polynomial of degree at most \( k \) in each dimension. Uniform grid: \( l_1 = l_2 = N \), \( V^k_l = V^k_N \), then

\[
V^k_N := V^k_{N,x_1} \times V^k_{N,x_2} = \bigoplus_{|l|_\infty \leq N} W^k_l
\]

where

\[
W^k_l := W^k_{l_1,x_1} \times W^k_{l_2,x_2}
\]

The basis functions for \( W^k_l \) can be defined by a tensor product

\[
v^{l_j}_{i,l}(x) := \prod_{t=1}^{2} v^{l_{t,j}}_{i_t,l_t}(x_t), \quad j_t = 0, \ldots, \max(0, 2^{l_t-1} - 1), \quad i_t = 1, \ldots, k + 1
\]
Full grid approximation space

Full grid space:

$$\mathbf{V}_N^k = \bigoplus_{|I|_\infty \leq N} \mathbf{W}_I^k$$

$$d = 2, \ N = 2, \ k = 0$$

\[
\begin{array}{c|c|c}
\hline
& W_{00} & W_{10} \\
\hline
1 & 1 & -1 \\
\hline
W_{01} & -1 & 1 \\
\hline
W_{02} & -\sqrt{2} & \sqrt{2} \\
\hline
W_{11} & 1 & -1 \\
\hline
W_{12} & \sqrt{2} & -\sqrt{2} \\
\hline
W_{21} & 1 & -1 \\
\hline
W_{22} & 2 & -2 \\
\hline
\end{array}
\]
Sparse grid approximation space

We consider the sparse grid space: \( \hat{V}_N^k := \bigoplus_{||l||_1 \leq N} W_l^k \)

A viewpoint without using multiwavelet space: \( \hat{V}_N^k = \bigoplus_{||l||_1 \leq N} V_l^k \).

\[ \text{dim}(\hat{V}_N^k) = O(2^N N^{d-1} (k + 1)^d) \quad \text{or} \quad O(h^{-1} |\log_2 h|^{d-1}) \]
Consider the linear transport equation with variable coefficient

\[
\begin{aligned}
    &u_t + \nabla \cdot (\alpha(x, t) u) = 0, \quad x \in \Omega = [0, 1]^d, \\
    &u(0, x) = u_0(x),
\end{aligned}
\]

The semi-discrete DG formulation for (1) is defined as follows: find \( u_h \in \hat{V}_N^k \), such that

\[
\int_\Omega (u_h)_t v_h \, dx = \int_\Omega u_h \alpha \cdot \nabla v_h \, dx - \sum_{e \in \Gamma} \int_e \hat{\alpha} u_h \cdot [v_h] \, ds,
\]

\[
\dot{=} A(u_h, v_h)
\]

for \( \forall v_h \in \hat{V}_N^k \), where \( \hat{\alpha} u_h \) defined on the element interface denotes a monotone numerical flux.
Stability (constant coefficient case)

Theorem ($L^2$ stability)

The DG scheme (2) for (1) is $L^2$ stable when $\alpha$ is a constant vector, i.e.

$$\frac{d}{dt} \int_{\Omega} (u_h)^2 \, dx = - \sum_{e \in \Gamma} \int_e \frac{|\alpha \cdot n|}{2} |[u_h]|^2 \, ds \leq 0. \quad (3)$$
Error estimate (constant coefficient case)

Similar to Schwab, Suli, Todor (08), we can establish error estimate in $L^2$ norm for the $L^2$ projection operator, combining with an estimate for DG method, we get

**Theorem ($L^2$ error estimate)**

Let $u$ be the exact solution, and $u_h$ be the numerical solution to the semi-discrete scheme (2) with numerical initial condition $u_h(0) = P u_0$. For $k \geq 1$, $u_0 \in \mathcal{H}^{p+1}(\Omega)$, $1 \leq q \leq \min\{p, k\}$, $N \geq 1$, $d \geq 2$, we have for all $t \geq 0$,

$$
\|u_h - u\|_{L^2(\Omega_N)} \leq \left( 2 \sqrt{C_d} \|\alpha\|_{2} t C_\star(k, q, d, N) + (\bar{c}_{k,0,q} + B_0(k, q, d) \kappa_0(k, q, N)^d) 2^{-N/2} \right) 2^{-N(q+1/2)} |u_0|_{\mathcal{H}^{q+1}(\Omega)},
$$

where $C_d$ is a generic constant with dependence only on $d$,

$$
C_\star(k, q, d, N) = \max_{s=0,1} (\bar{c}_{k,s,q} + B_s(k, q, d) \kappa_s(k, q, N)^d).
$$

The constants $\bar{c}_{k,s,q}$, $B_s(k, q, d)$, $\kappa_s(k, q, N)$ are defined in $L^2$ projection error estimates.

Convergence rate $O((\log h)^d h^{k+1/2})$. 

Adaptivity

To resolve fine local structures/accelerate the computation

- Adaptive DG methods.
- Adaptive sparse grid schemes. Zenger (90), Griebel (98), Bokanowski et al. (12)...
- Multiresolution finite difference/finite volume methods for hyperbolic PDEs. Harten (95), Bihari, Harten (97), Dahmen et al. (01), Cohen et al. (03)
- Adaptive multiresolution DG schemes Calle et al. (2005), Archibald et al. (2011), Hovhannisyan et al. (2014), Gerhard et al. (2015)
Refinement criteria

For a function \(u(x) \in \mathcal{H}^{p+1}(\Omega)\), we can show that
\[
u(x) = \sum_{l \in \mathbb{N}_0} \sum_{j \in B_l, 1 \leq i \leq k+1} u_{i,l}^j v_{i,l}^j(x),
\]
where the hierarchical coefficient is
\[
u_{i,l}^j = \int_\Omega u(x) v_{i,l}^j(x) \, dx.
\]
An element \(V_{i,l}^j := \{v_{i,l}^j, 1 \leq i \leq k + 1\}\) is considered important if
\[
\sum_{1 \leq i \leq k+1} |u_{i,l}^j| \|v_{i,l}^j(x)\|_{L^1(\Omega)} > \varepsilon, \quad \text{if} \quad s = 1
\]
\[
\left( \sum_{1 \leq i \leq k+1} |u_{i,l}^j|^2 \right)^{\frac{1}{2}} > \varepsilon, \quad \text{if} \quad s = 2
\]
\[
\sum_{1 \leq i \leq k+1} |u_{i,l}^j| \|v_{i,l}^j(x)\|_{L^\infty(\Omega)} > \varepsilon, \quad \text{if} \quad s = \infty,
\]
where \(\varepsilon\) is a prescribed error threshold.
A similar coarsening criteria can be defined.
Adaptive evolution algorithm

Input: Hash table $H$ and leaf table $L$ at $t^n$, numerical solution $u_h^n \in V_{N,H}^k$.  
Parameters: Maximum level $N$, polynomial degree $k$, error constants $\varepsilon, \eta$, CFL constant.  
Output: Hash table $H$ and leaf table $L$ at $t^{n+1}$, numerical solution $u_h^{n+1} \in V_{N,H}^k$.

- **Prediction.** Given a hash table $H$ that stores the numerical solution $u_h$ at time step $t^n$, calculate $\Delta t$. Predict the solution by the DG scheme using space $V_{N,H}^k$ and the forward Euler time stepping method. Generate the predicted solution $u_h^{(p)}$.  

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Adaptive evolution algorithm

- **Refinement.** Based on the predicted solution $u_h^{(p)}$, screen all elements in the hash table $H$. If for element $V_i^j$, the refining criteria hold, then add its children elements to $H$ and $L$ provided they are not added yet, and set the associated detail coefficients to zero. We also need to make sure that all the parent elements of the newly added element are in $H$ (i.e., no “hole” is allowed in the hash table) and increase the number of children for all its parent elements by one. This step generates the updated hash table $H^{(p)}$ and leaf table $L^{(p)}$. 
Adaptive evolution algorithm

- **Evolution.** Given the predicted table $H(p)$ and the leaf table $L(p)$, we evolve the solution from $t^n$ to $t^{n+1}$ by the DG scheme using space $V_{N,H(p)}^k$ and the third order Runge-Kutta time stepping method. This step generates the pre-coarsened numerical solution $\tilde{u}_h^{n+1}$.

- **Coarsening.** For each element in the leaf table, if the coarsening criteria hold, then remove the element from table $H(p)$ and $L(p)$. For each of its parent elements in $H(p)$, we decrease the number of children by one. If the number becomes zero, i.e., the element has no child, then it will be added to leaf table $L(p)$. Repeat the coarsening procedure until no element can be removed from the leaf list. Denote the resulting hash table and leaf table by $H$ and $L$ respectively, and the compressed numerical solution $u_h^{n+1} \in V_{N,H}^k$. 
We consider the following linear advection problem

\[
\begin{aligned}
    & u_t + \sum_{m=1}^{d} u_{x_m} = 0, \quad \mathbf{x} \in [0, 1]^d, \\
    & u(0, \mathbf{x}) = \sin \left( 2\pi \sum_{m=1}^{d} x_m \right),
\end{aligned}
\]  

(7)

subject to periodic boundary conditions.

In the simulation, we compute the numerical solutions up to two periods in time, meaning that we let final time \( T = 1 \) for \( d = 2 \), \( T = 2/3 \) for \( d = 3 \), and \( T = 0.5 \) for \( d = 4 \).
Table: $L^2$ errors and orders of accuracy at $T = 1$ when $d = 2$, $T = 2/3$ when $d = 3$, and $T = 0.5$ when $d = 4$. $N$ is the number of mesh levels, $h_N$ is the size of the smallest mesh in each direction, $k$ is the polynomial order, $d$ is the dimension. DOF denotes the degrees of freedom of the sparse approximation space $\hat{V}_N^k$. $L^2$ order is calculated with respect to $h_N$.

<table>
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<tr>
<th>$N$</th>
<th>$h_N$</th>
<th>$k = 1, d = 2$</th>
<th>$k = 1, d = 3$</th>
<th>$k = 1, d = 4$</th>
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<td></td>
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<td>DOF</td>
<td>$L^2$ error</td>
<td>order</td>
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<tr>
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<td>1/32</td>
<td>448</td>
<td>1.90E-02</td>
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</tr>
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<td>6</td>
<td>1/64</td>
<td>1024</td>
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<td>1/128</td>
<td>2304</td>
<td>1.27E-03</td>
<td>1.92</td>
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<td></td>
</tr>
<tr>
<td>4</td>
<td>1/16</td>
<td>432</td>
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<td>–</td>
</tr>
<tr>
<td>5</td>
<td>1/32</td>
<td>1008</td>
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<td>3</td>
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<td>320</td>
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<td>9216</td>
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</table>
We test the convergence of adaptive scheme with smooth initial
\[ u(0, x) = \prod_{m=1}^{d} \sin^4(\pi x_m). \]
For smooth case, we fix \( N = 7 \), and calculate

convergence rate with respect to \( \varepsilon \)
\[ R_{\varepsilon_l} = \frac{\log(e_{l-1}/e_l)}{\log(\varepsilon_{l-1}/\varepsilon_l)}. \]

convergence rate with respect to DOF
\[ R_{\text{DOF}_l} = \frac{\log(e_{l-1}/e_l)}{\log(\text{DOF}_l/\text{DOF}_{l-1})}. \]
Table: Numerical error and convergence rate. $N = 7$. $T = 1$. $L^2$ norm based criteria.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>DOF</th>
<th>$L^2$ error</th>
<th>$R_{DOF}$</th>
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Linear advection: discontinuous profile

We consider

\[
  u(0, x) = \begin{cases} 
    1 & (x_1, x_2) \in \left[\frac{1}{2} - \frac{\sqrt{6}}{2}, \frac{1}{2} + \frac{\sqrt{6}}{2}\right]^2, \\
    0 & \text{otherwise},
  \end{cases}
\]  

(8)

We fix \( N = 7, \varepsilon = 10^{-5} \) and compare the performance of the scheme with \( L^1, L^2 \) and \( L^\infty \) based refinement/coarsening criteria up to final time \( T = 1 \).
(c) $L^2$ criteria: solution

(d) $L^2$ criteria: active elements

(e) $L^\infty$ criteria: solution

(f) $L^\infty$ criteria: active elements
Kinetic simulations: background

- Kinetic simulations are in high dimension because of the need to resolve the probability distribution functions.
- Numerical methods should be designed with computational efficiency, and also maintain key properties of the solutions.
- DG methods have been developed to compute Vlasov equations and Boltzmann equations. They are known for their excellent conservation properties, see Gamba et al.
- Sparse grid methods for kinetic problems have been developed in the literature, e.g. wavelet-MRA method Besse et al (08); sparse adaptive FEM Widmer et al (98); sparse discrete ordinate method, sparse tensor spherical harmonics Grella, Schwab (11); combination techniques for linear gyrokinetics Kowtiz et al (13).
- Here, we consider the Vlasov-Poisson system, for which the solution is known to develop filamentations (fine scale structures).
Vlasov-Poisson simulation

We consider

$$f_t + \mathbf{v} \cdot \nabla_x f + \mathbf{E}(t, \mathbf{x}) \cdot \nabla_v f = 0,$$

$$-\Delta_x \Phi(\mathbf{x}) = \rho - 1, \quad \mathbf{E}(\mathbf{x}) = -\nabla_x \Phi$$

where $f(t, \mathbf{x}, \mathbf{v})$ denotes the probability distribution function of electrons. $\mathbf{E}(t, \mathbf{x})$ is the self-consistent electrostatic field given by Poisson’s equation (10) and

$$\rho(t, \mathbf{x}) = \int_v f(t, \mathbf{x}, \mathbf{v}) d\mathbf{v}$$

denotes the electron density. Ions are assumed to form a neutralizing background.

- **Landau damping:**

  $$f(0, \mathbf{x}, \mathbf{v}) = f_M(\mathbf{v})(1 + A \cos(kx)), \quad x \in [0, L], \quad \mathbf{v} \in [-V_c, V_c],$$

  where $A = 0.5$, $k = 0.5$, $L = 4\pi$, $V_c = 2\pi$, and $f_M(\mathbf{v}) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}$.

- **Bump-on-tail instability:**

  $$f(0, \mathbf{x}, \mathbf{v}) = f_{BT}(\mathbf{v})(1 + A \cos(kx)), \quad x \in [0, L], \quad \mathbf{v} \in [-V_c, V_c],$$

  where $A = 0.04$, $k = 0.3$, $L = 20\pi/3$, $V_c = 13$, and

  $$f_{BT}(\mathbf{v}) = n_p \exp \left( -\frac{\mathbf{v}^2}{2} \right) + n_b \exp \left( -\frac{|\mathbf{v} - \mathbf{u}|^2}{2\nu_t^2} \right),$$

  where $n_p = \frac{9}{10\sqrt{10\pi}}$, $n_b = \frac{2}{10\sqrt{10\pi}}$, $\mathbf{u} = 4.5$, $\nu_t = 0.5$. 
Vlasov-Poisson simulation

- **Two-stream instability I:**
  \[
  f(0, x, v) = f_{TSI}(v)(1 + A \cos(kx)), \quad x \in [0, L], \ v \in [-V_c, V_c],
  \]
  where \( A = 0.05, \ k = 0.5, \ L = 4\pi, \ V_c = 2\pi, \text{ and } \)
  \[
  f_{TSII}(v) = \frac{1}{\sqrt{2\pi}} v^2 e^{-v^2/2}.
  \]

- **Two-stream instability II:**
  \[
  f(0, x, v) = f_{TSII}(v)(1 + A \cos(kx)), \quad x \in [0, L], \ v \in [-V_c, V_c],
  \]
  where \( A = 0.05, \ k = 2/13, \ L = 13\pi, \ V_c = 5, \text{ and } \)
  \[
  f_{TSII}(v) = \frac{1}{2v_t \sqrt{2\pi}} \left( \exp \left( -\frac{|u + v|^2}{2v_t^2} \right) + \exp \left( -\frac{|u - v|^2}{2v_t^2} \right) \right),
  \]
  where \( u = 0.99, \ v_t = 0.3. \)
Conservation properties of moments for sparse grid DG

- $1, |\mathbf{v}|^2$ still belongs to the space $\hat{V}_N^k$ when $k \geq 2$. That’s the key to particle number and energy conservation.
- If one wants to design a DG scheme with particle number and energy conservation, it is key to choose a basis set that includes $1$ and $|\mathbf{v}|^2$ on level 0, while on other levels the bases can be chosen freely according to accuracy consideration.
- Conservation for adaptive sparse grids will deteriorate due to the error contribution at velocity domain boundary.
Conservation: Landau damping (sparse grid DG)
Conservation: adaptive sparse grid DG
Applications in kinetic simulations

Comparison: two stream instability I

(o) Sparse grid DG

(p) Adaptive multiresolution DG $\varepsilon = 10^{-5}$

Figure: $T = 10$, $k = 3$, $N = 7$
Applications in kinetic simulations

Comparison: two stream instability I

(a) Sparse grid DG

(b) Adaptive multiresolution DG $\varepsilon = 10^{-5}$

Figure: $T = 20, k = 3, N = 7$
Conclusion and future work

- The sparse grid DG can save storage and computation cost as the size of approximation spaces are significantly reduced from the standard exponential dependence $O(h^{-d})$ to $O(h^{-1}|\log_2 h|^{d-1})$.

- $L^2$ stability and error estimates of order $O((\log h)^d h^{k+1/2})$ are established. Numerical error is only slightly deteriorated for smooth solutions.

- Similar conservation and stability properties hold when compared with traditional DG spaces.

- Adaptivity can be incorporated automatically capture fine local structures, capturing less regular solutions.

- Future work: nonlinear equations, other applications, hp adaptivity...
Happy Birthday, Irene!

Thank you for everything!