A sparse grid discontinuous Galerkin method for high-dimensional transport equations

Wei Guo

Michigan State University
Joint work with Yingda Cheng

National Center for Atmospheric Research
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Consider the following scalar transport equation

\[
\begin{align*}
\frac{\partial u}{\partial t} + \nabla \cdot \left( \alpha(u, x, t) u \right) &= 0, \quad x \in \Omega = [0, 1]^d, \\
u(0, x) &= u_0(x).
\end{align*}
\]

- \( \alpha \): velocity field depending on \( x, t, \) and \( u \);
- \( d > 3 \): high dimensionality;
- wide range of applications
  - kinetic models: Vlasov equation, Boltzmann equation, radiative transfer, among others.
  - mathematical finance...
Example: Vlasov-Poisson system

A collisionless plasma can be described by the nonlinear Vlasov-Poisson system:

\[ f_t + \mathbf{v} \cdot \nabla_x f + \mathbf{E} \cdot \nabla_v f = 0, \]
\[ \mathbf{E} = -\nabla_x \phi, \quad -\Delta_x \phi = \rho - 1. \]

- \( f(t, x, v) \): the probability of finding a particle with velocity \( v \) at position \( x \) at time \( t \).
- \( \mathbf{E} \): electric field.
- \( \rho = \int f \, dv \): the macroscopic charge density.
Challenges of the Vlasov-Poisson simulation

- High dimensionality of the Vlasov equation: $6D + \text{time}$.
- Multiple scales in space: filamentation.

**Figure:** Landau damping.
Outline

1. Sparse grid discontinuous Galerkin (DG) method

2. An adaptive multiresolution DG method
Outline

1. Sparse grid discontinuous Galerkin (DG) method

2. An adaptive multiresolution DG method
DG method: a review

- DG methods belong to the class of finite element methods, have been well developed since 1970s.
- **Curse of dimensionality**: the computational cost and storage requirements scale like $O(h^{-d})$ for a $d$-dimensional problem. $h$: the mesh size.
Sparse grid

Sparse grid: breaking the curse of dimensionality.

- Inspired by sparse grid quadrature Smolyak (63), introduced by Zenger (91), developed by Griebel (91,98,05...).

- When solving high-dimensional PDEs, sparse grid method has been incorporated in finite volume methods Hemker (95); finite difference methods: Griebel (98), Griebel, Zumbusch (99); finite element methods: Bungartz, Griebel (04), Schwab et al. (08); and spectral methods: Griebel (07), Gradinaru (07), Shen, Wang (10), Shen, Yu (10).

- Goal: explore the potential of the sparse grid technique in the DG framework for solving the Vlasov equation efficiently.
Hierarchical decomposition of piecewise polynomial spaces

Consider $\Omega = [0, 1]:$

$$\Omega_0 \quad 0 \quad \cdots \quad 1 \quad V_0^k : \text{polynomial space on } \Omega_0$$

- Nested structure:
  $$V_0^k \subset V_1^k \subset V_2^k \subset V_3^k \subset \cdots$$

- $W_n^k$: $L^2$ orthogonal complement of $V_{n-1}^k$ in $V_n^k$ for $n > 1$, i.e.,
  $$V_{n-1}^k \oplus W_n^k = V_n^k \quad \text{and} \quad W_n^k \perp V_{n-1}^k.$$
Hierarchical decomposition of piecewise polynomial spaces

Consider $\Omega = [0, 1]$:

\[
\begin{align*}
\Omega_0 & \quad \begin{array}{c}
0 \quad \longrightarrow \quad 1
\end{array} \quad V^k_0 : \text{polynomial space on } \Omega_0 \\
\Omega_1 & \quad \begin{array}{c}
0 \quad \longrightarrow \quad 1
\end{array} \quad V^k_1 : \text{piecewise polynomial space on } \Omega_1
\end{align*}
\]

- Nested structure:
  \[ V^k_0 \subset V^k_1 \subset V^k_2 \subset V^k_3 \subset \cdots \]

- $W^k_n$: $L^2$ orthogonal complement of $V^{k}_{n-1}$ in $V^k_n$ for $n > 1$, i.e.,
  \[ V^k_{n-1} \oplus W^k_n = V^k_n \quad \text{and} \quad W^k_n \perp V^k_{n-1}. \]
Hierarchical decomposition of piecewise polynomial spaces

Consider $\Omega = [0, 1]$: 

- $V_0^k$: polynomial space on $\Omega_0$
- $V_1^k$: piecewise polynomial space on $\Omega_1$
- $V_2^k$: piecewise polynomial space on $\Omega_2$

Nested structure:

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

- $W_n^k$: $L^2$ orthogonal complement of $V_{n-1}^k$ in $V_n^k$ for $n > 1$, i.e.,

$$V_{n-1}^k \oplus W_n^k = V_n^k \quad \text{and} \quad W_n^k \perp V_{n-1}^k.$$
Hierarchical decomposition of piecewise polynomial spaces

Consider $\Omega = [0, 1]$

$$\begin{align*}
\Omega_0 & \quad 0 \quad 1 \quad V_0^k \\
\Omega_1 & \quad 0 \quad 1 \quad V_1^k = V_0^k \oplus W_1^k \\
\Omega_2 & \quad 0 \quad 1 \quad V_2^k = V_1^k \oplus W_2^k \\
\end{align*}$$

- Nested structure:
  $$V_0^k \subset V_1^k \subset V_2^k \subset V_3^k \subset \cdots$$
- $W_n^k$: $L^2$ orthogonal complement of $V_{n-1}^k$ in $V_n^k$ for $n > 1$, i.e.,
  $$V_{n-1}^k \oplus W_n^k = V_n^k \quad \text{and} \quad W_n^k \perp V_{n-1}^k.$$
\( V_{n-1} \oplus W_n^k = V_n^k \)

- \( W_n^k \) is called the increment space and represents the finer level details when the mesh is refined.
- Define \( W_0^k := V_0^k \), then

\[
V_N^k = \bigoplus_{0 \leq n \leq N} W_n^k ,
\]

where \( N \) is the maximum mesh level. \( V_N^k \) is decomposed in terms of increment spaces \( W_n^k \).
Background for multiwavelet

Multiwavelet: multi-scale bases of the increment spaces.

- Haar wavelet \((k = 0)\) Haar (1910).
- \(L^2\) orthogonal multiwavelet bases \((k \geq 1)\) Alpert (1993).
Hierarchical orthonormal bases (Alpert’s multiwavelet)

Bases in $W_0^k$: scaled orthonormal Legendre polynomials.

Bases in $W_1^k$: mother wavelet

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

The orthonormal, vanishing-moment functions $\{f_i(x)\}_k$ (Alpert 93).

Bases in $W_n^k$, $n \geq 1$:

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

Orthonormality of multiwavelet bases across different hierarchical levels

$$\int_0^1 v_{i,n}^j(x) v_{i',n'}^{j'}(x) \, dx = \delta_{ii'} \delta_{nn'} \delta_{jj'}.$$
Multiwavelets on different levels

- $k = 0$: Haar wavelet

\[ \Omega_0 = 1 \quad W_0^0 \quad \text{dim}(W_0^0) = 1 \]

\[ \Omega_1 = 1 \quad W_1^0 \quad \text{dim}(W_1^0) = 1 \]

\[ \Omega_2 = \sqrt{2} \quad W_2^0 \quad \text{dim}(W_2^0) = 2 \]
Multiwavelets on different levels

- $k = 1$:

  - $\Omega_0$
    - $\sqrt{3}$
    - $-\sqrt{3}$
    - $1$
  - $\Omega_1$
    - $\sqrt{3}$
    - $-\sqrt{3}$
    - $2$
    - $-1$
    - $-2$
  - $\Omega_2$
    - $\sqrt{6}$
    - $-\sqrt{6}$
    - $2\sqrt{2}$
    - $-\sqrt{2}$
    - $-2\sqrt{2}$

- $W_0^1$, $\dim(W_0^1) = 2$
- $W_1^1$, $\dim(W_1^1) = 2$
- $W_2^1$, $\dim(W_2^1) = 4$
Full grid approximation space in multi-dimensions

Full grid space: \( \mathbf{V}_N^k := \mathbf{V}_{N,x_1}^k \times \ldots \times \mathbf{V}_{N,x_d}^k = \bigoplus_{|\mathbf{n}|_\infty \leq N} \mathbf{W}_n^k, \)

where \( \mathbf{W}_n^k = W_{n_1,x_1}^k \times \ldots \times W_{n_d,x_d}^k, \quad \mathbf{n} = (n_1, \ldots, n_d), \quad |\mathbf{n}|_\infty = \max(n_1, \ldots, n_d). \)

\( d = 2, \ N = 2, \ k = 0: \)

Tensor product bases: \( \nu_{i,n}^j(x) := \prod_{m=1}^{d} \nu_{i,m,n_m}^j(x_m). \)
Sparse grid approximation space

Sparse grid space by truncation:

\[ \hat{V}_k^N := \bigoplus_{|n|_1 \leq N} W_n^k, \quad \text{with} \quad |n|_1 = n_1 + \ldots + n_d, \quad \hat{V}_k^N \subset V_k^N. \]

\[ d = 2, \; N = 2, \; k = 0: \quad \]

\[ \begin{array}{cccc}
1 & 1 & \sqrt{2} & -\sqrt{2} \\
-1 & -1 & -\sqrt{2} & \sqrt{2} \\
\end{array} \]

\[ \begin{array}{cccc}
W_{00} & W_{10} & W_{20} \\
-1 & 1 & -\sqrt{2} \sqrt{2} \sqrt{2} \\
1 & -1 & \sqrt{2} \sqrt{2} \sqrt{2} \\
\end{array} \]

\[ \begin{array}{cccc}
W_{01} & W_{11} \\
-1 & 1 \\
1 & -1 \\
\end{array} \]

\[ \begin{array}{cccc}
W_{02} \\
-\sqrt{2} \sqrt{2} \sqrt{2} \sqrt{2} \\
\end{array} \]
**DOF comparison: sparse grid $\hat{V}_N^k$ vs. full grid $V_N^k$**

**Lemma:** $\dim(\hat{V}_N^k) = O(h^{-1} \log_2 h^{d-1})$ vs. $\dim(V_N^k) = O(h^{-d})$, $h = 2^{-N}$.

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 Approximation properties of $\hat{V}^k_N$

Lemma (G. and Cheng (16))

Let $P$ be the standard $L^2$ projection onto the space $\hat{V}^k_N$, then for $k \geq 1$, $N \geq 1$, $d \geq 2$, and any $v \in \mathcal{H}^{p+1}(\Omega)$, $1 \leq q \leq \min\{p, k\}$, we have

$$|Pv - v|_{H^s(\Omega_N)} \lesssim \begin{cases} 
N^d 2^{-N(q+1)}|v|_{\mathcal{H}^{q+1}(\Omega)} & s = 0, \\
2^{-Nq}|v|_{\mathcal{H}^{q+1}(\Omega)} & s = 1.
\end{cases}$$

Since $h = 2^{-N}$, if the solution is sufficiently smooth, the projection error scales as

- $O(|\log_2 h|^d h^{k+1})$ in $L^2$ norm,
- $O(h^k)$ in broken $H^1$ semi-norm.

Nothing comes for free: mixed derivative semi-norm $|\cdot|_{\mathcal{H}^{q+1}}$ is stronger than $|\cdot|_{H^{q+1}}$. 
Consider the linear transport equation with variable coefficient

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

(3)

The semi-discrete sparse grid DG formulation for (3) is defined as follows: find \( u_h \in \hat{V}_N^k \), such that

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

(4)

for \( \forall v_h \in \hat{V}_N^k \), where \( \hat{\alpha} u_h \) defined on the element interface \( e \) denotes a monotone numerical flux. \([v_h]\) denotes the jump of \( v_h \) on \( e \).

* The same weak formulation as the traditional DG method.
Stability (constant coefficient case)

Theorem ($L^2$ stability)

The DG scheme (4) for (3) is $L^2$ stable when $\alpha$ is a constant vector, i.e.

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

**Theorem** ($L^2$ error estimate, G. and Cheng (16))

Let $u$ be the exact solution to (5), and $u_h$ be the numerical solution to the semi-discrete scheme (4) with numerical initial condition $u_h(0) = Pu_0$. For $k \geq 1$, $u \in \mathcal{H}^{p+1}(\Omega)$, $1 \leq q \leq \min\{p, k\}$, $N \geq 1$, $d \geq 2$, we have for all $t \geq 0$,

$$\|u_h - u\|_{L^2(\Omega)} \lesssim \left(\sqrt{t} + 2^{-N/2}\right) N^d 2^{-N(q+1/2)} |u|_{\mathcal{H}^{q+1}(\Omega)}.$$  

Convergence rate $O(\|\log_2 h\|^d h^{k+1/2})$ if $u$ is sufficiently smooth.
Numerical test: linear advection with constant coefficient

Consider the following linear advection problem

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

(5)

with 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 \( d = 4 \).
- A third order strong stability preserving Runge-Kutta method is used for time integration.
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Convergence rate $O(|\log h|^d h^{k+1/2})$. 
Summary so far

- Major advantages of the sparse grid DG scheme
  - low computational and storage cost;
  - accuracy is only slightly deteriorated for smooth problems;
  - provable stability and convergence properties.

- Requires a strong smoothness assumption of the solution.
  *A priori* type of choice of the sparse grid approximation space, e.g. $|n|_1 \leq N$ is not optimal.

- We develop a novel adaptive multiresolution scheme
  - becomes a sparse grid DG method when the solution is smooth;
  - can automatically capture localized fine structures.
Outline

1. Sparse grid discontinuous Galerkin (DG) method

2. An adaptive multiresolution DG method
An adaptive multiresolution DG method

Adaptive multiresolution DG method (G. and Cheng (16))

Multiwavelet expansion

\[ u_h(x) = \sum_{n,j,i} u_{i,n}^j v_{i,n}^j(x). \]

The adaptive multiresolution DG method

- measures the multiwavelet coefficients \( u_{i,n}^j \) as a natural error indicator,
- uses \( \varepsilon \)-thresholding for refinement or coarsening. When \( k = 0 \),
  - \( |u_{i,n}^j| > \varepsilon \): significant element, local refinement is required;
  - \( |u_{i,n}^j| < \varepsilon \): insignificant element, discard for efficiency.

In implementation,

- a hash table is adopted as the underlying data structure;
- we follow the standard adaptive paradigm
  
  predict \( \rightarrow \) mark \( \rightarrow \) refine \( \rightarrow \) evolve \( \rightarrow \) coarsen

to keep track of the significant elements over time evolution.
Consider the 2D deformational flow with velocity field

$$\alpha = (\sin^2(\pi x_1) \sin(2\pi x_2) g(t), -\sin^2(\pi x_2) \sin(2\pi x_1) g(t)),$$

where $g(t) = \cos(\pi t / T)$ with $T = 1.5$.

- Along the direction of the flow, the initial condition will be quite deformed at $t = T/2$, then go back to its initial state at $t = T$ as the flow reverses.
- Consider two initial conditions: a smooth cosine bell and a discontinuous step function.
Accuracy test

- Convergence rate with respect to DOF: \( R_{\text{DOF}} = \frac{\log(e_{l-1}/e_l)}{\log(\text{DOF}_l/\text{DOF}_{l-1})} \).

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

Table: Smooth initial condition. Numerical error and convergence rate. \( N = 7 \). \( T = 1.5 \).

<table>
<thead>
<tr>
<th>( \varepsilon )</th>
<th>DOF</th>
<th>( L^2 ) error</th>
<th>( R_{\text{DOF}} )</th>
<th>( R_{\varepsilon} )</th>
<th>DOF</th>
<th>( L^2 ) error</th>
<th>( R_{\text{DOF}} )</th>
<th>( R_{\varepsilon} )</th>
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<tbody>
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<td>( k = 2 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>( k = 3 )</td>
<td></td>
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<td></td>
</tr>
<tr>
<td>5E-05</td>
<td>1143</td>
<td>5.41E-04</td>
<td>-</td>
<td>-</td>
<td>1056</td>
<td>3.65E-04</td>
<td>-</td>
<td>-</td>
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<tr>
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<td>1.15E-04</td>
<td>2.67</td>
<td>0.96</td>
<td>2048</td>
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<td>2.14</td>
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<td>5.41E-05</td>
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<tr>
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<td>0.82</td>
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<td>1.90</td>
<td>0.59</td>
<td>4480</td>
<td>6.32E-06</td>
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<td>3.82</td>
<td>1.16</td>
</tr>
</tbody>
</table>

- \( R_{\text{DOF}} \) for the adaptive scheme is much larger than \( R_{\text{DOF}} = \frac{k+1}{d} \) for the full grid DG scheme.
- \( R_{\varepsilon} \approx 1 \).
Figure: Discontinuous step function. $N = 7$, $k = 3$, $\varepsilon = 10^{-5}$. 
Two benchmark tests in 1D1V:

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

- **Bump-on-tail instability:**
  \[ f(0, x, v) = f_{BT}(v)(1 + A \cos(kx)), \quad x \in [0, L], \ v \in [-V_c, V_c], \]
  where \( A = 0.04, \ k = 0.3, \ L = \frac{20\pi}{3}, \ V_c = 13, \) and
  \[ f_{BT}(v) = n_p \exp \left(-\frac{v^2}{2}\right) + n_b \exp \left(-\frac{|v - u|^2}{2v_t^2}\right), \]
  where \( n_p = \frac{9}{10\sqrt{10\pi}}, \ n_b = \frac{2}{10\sqrt{10\pi}}, \ u = 4.5, \ v_t = 0.5. \)
An adaptive multiresolution DG method

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Figure: Two-stream instability. $T = 20$, $N = 7$, $k = 3$. Sparse grid DG: DOF = 9216; adaptive DG: DOF = 45792; full grid DG: DOF = 262144.
Table: Comparison between the proposed adaptive scheme and the full grid method for the two-stream instability. The solution difference in $L^2$ norm at $t = 1$, $t = 10$, $t = 20$ and $t = 40$. $N = 7$. $k = 3$.

<table>
<thead>
<tr>
<th>$\varepsilon$</th>
<th>$t = 1$</th>
<th>$t = 10$</th>
<th>$t = 20$</th>
<th>$t = 40$</th>
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<tr>
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<tr>
<td>1E-06</td>
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<td>1.94E-04</td>
<td>1.97E-04</td>
<td>4.58E-04</td>
</tr>
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</table>
Bump-on-tail instability. $N = 7$, $k = 3$, $\varepsilon = 10^{-5}$.
Conclusion

- 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.

- An adaptive multi-resolution DG method is developed, which is able to become a sparse grid DG method when the solution is smooth and automatically capture localized fine structures.

- Future work and challenges:
  - theoretical investigation for the adaptive scheme;
  - implementation for the high-dimensional Vlasov equation;
  - extension to other equations: Vlasov-Maxwell system, Wigner-Poisson system, radiative transfer,....


Any questions?
Thank You!


Relaxation model

\[ f_t + \mathbf{v} \cdot \nabla_x f + \mathbf{E}(t, \mathbf{x}) \cdot \nabla_v f = \frac{\mu_\infty(\mathbf{v}) \rho(t, \mathbf{x}) - f(t, \mathbf{x}, \mathbf{v})}{\tau}, \]

where

\[ \mu_\infty(\mathbf{v}) = \frac{\exp\left(-\frac{|\mathbf{v}|^2}{2\theta}\right)}{(2\pi\theta)^{d/2}}, \]

and

\[ \rho(t, \mathbf{x}) = \int f(t, \mathbf{x}, \mathbf{v}) \, d\mathbf{v} \]

denotes the macroscopic density. The external electric field \( \mathbf{E}(t, \mathbf{x}) \) is given by

\[ \mathbf{E}(\mathbf{x}) = -\nabla_x \Phi(\mathbf{x}) \quad \text{with} \quad \Phi(\mathbf{x}) = \frac{|\mathbf{x}|^2}{2}. \]

Global Maxwellian distribution

\[ \mathcal{M}(\mathbf{x}, \mathbf{v}) = \rho_\infty(\mathbf{x}) \mu_\infty(\mathbf{v}) = \frac{\exp\left(-\left(\frac{|\mathbf{v}|^2}{2} + \Phi(\mathbf{x})\right)/\theta\right)}{(2\pi\theta)^{d/2} \int_x \exp(-\Phi(\mathbf{x})/\theta) \, d\mathbf{x}}. \]
Figure: The two-dimensional cuts in $x_1 - v_1$ plane of the evolution of $f_h$ towards equilibrium at $x_2 = 0$ and $v_2 = 0$. $t = 0$ (a), $t = 0.5$ (b), $t = 1$ (c), $t = 2$ (d), $t = 3$ (e), and $t = 6$ (f). $k = 3$, $N = 8$. 