Topic: Modeling and Numerical Simulation for Rarefied Gases

Lecture 3: Iterative Methods for Steady-State Boltzmann Equation

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2 Jul 2026

1 Fixed-point iteration for the Broadwell model

2 Symmetric Gauss-Seidel Method for the Broadwell equation

3 Acceleration of inner iterations

4 Symmetric Gauss-Seidel method for the Boltzmann equation

5 Summary

Dense gases

Boltzmann equation:

$$\partial_t f + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = Q(f, f)$$

When f is large, we let $f' = \varepsilon f$ and obtain

$$\partial_t f' + \boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f' = \frac{1}{\varepsilon} Q(f', f').$$

Below we will omit the prime and focus on the steady-state problem

$$\boldsymbol{v} \cdot \nabla_{\boldsymbol{x}} f = \frac{1}{\varepsilon} Q(f, f).$$

Review of the fixed-point iteration

Fixed-point iteration:

$$\boldsymbol{v}\cdot\nabla_{\boldsymbol{x}} f^{(k+1)} + \frac{\nu^{(k)}}{\varepsilon} f^{(k+1)} = \frac{1}{\varepsilon} Q(f^{(k)}, f^{(k)}) + \frac{\nu^{(k)}}{\varepsilon} f^{(k)},$$

where $\nu^{(k)}$ is chosen such that $Q(f^{(k)}, f^{(k)}) + \nu^{(k)} f^{(k)} \geq 0$.

The convergence is slow when ε is small!

Review of the Broadwell model

Broadwell model:

$$\begin{aligned}
\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= \sigma(wz - uv),\\
\frac{\partial v}{\partial t} - \frac{\partial v}{\partial x} &= \sigma(wz - uv),\\
\frac{\partial w}{\partial t} + \frac{\partial w}{\partial y} &= \sigma(uv - wz),\\
\frac{\partial z}{\partial t} - \frac{\partial z}{\partial y} &= \sigma(uv - wz).
\end{aligned}$$

We assume $\sigma = 1/\varepsilon$.

Review of the Broadwell model

Broadwell model:

$$\begin{aligned}
\frac{\partial u}{\partial x} &= \sigma(wz - uv), \\
-\frac{\partial v}{\partial x} &= \sigma(wz - uv), \\
\frac{\partial w}{\partial y} &= \sigma(uv - wz), \\
-\frac{\partial z}{\partial y} &= \sigma(uv - wz).
\end{aligned}$$

We assume $\sigma = 1/\varepsilon$.

Fixed-point iteration for the Broadwell model

Fixed-point iteration: Let $m = u + v + w + z$.

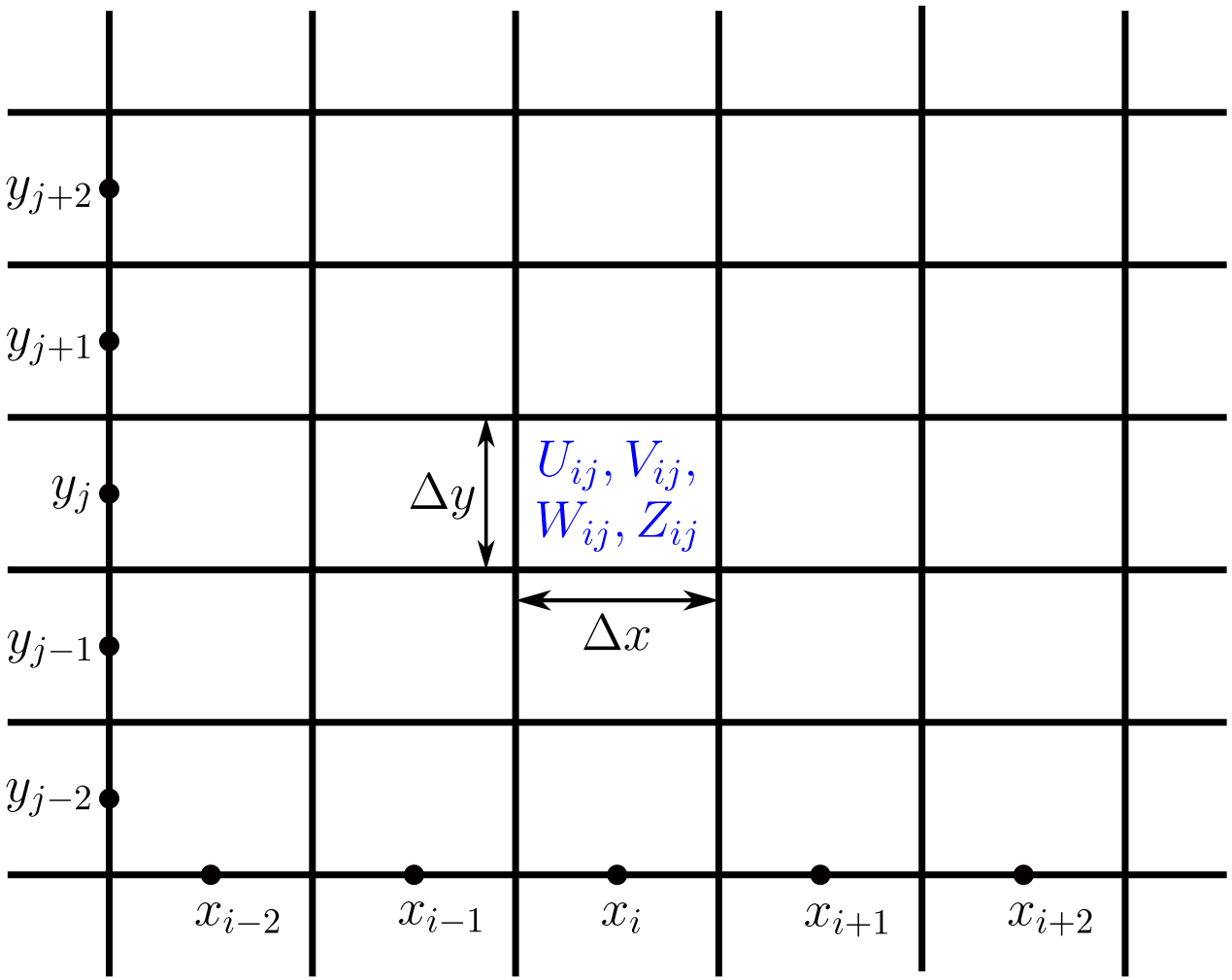
$$\sigma m^{(k)} u^{(k+1)} + \frac{\partial u^{(k+1)}}{\partial x} = \sigma(w^{(k)} z^{(k)} - u^{(k)} v^{(k)} + m^{(k)} u^{(k)}),$$

$$\sigma m^{(k)} v^{(k+1)} - \frac{\partial v^{(k+1)}}{\partial x} = \sigma(w^{(k)} z^{(k)} - u^{(k)} v^{(k)} + m^{(k)} v^{(k)}),$$

$$\sigma m^{(k)} w^{(k+1)} + \frac{\partial w^{(k+1)}}{\partial y} = \sigma(u^{(k)} v^{(k)} - w^{(k)} z^{(k)} + m^{(k)} w^{(k)}),$$

$$\sigma m^{(k)} z^{(k+1)} - \frac{\partial z^{(k+1)}}{\partial y} = \sigma(u^{(k)} v^{(k)} - w^{(k)} z^{(k)} + m^{(k)} z^{(k)}).$$

Spatial discretization



Spatial discretization

Upwind scheme:

$$\begin{aligned}
\frac{U_{ij} - U_{i-1,j}}{\Delta x} &= \sigma(W_{ij}Z_{ij} - U_{ij}V_{ij}),\\
\frac{V_{ij} - V_{i+1,j}}{\Delta x} &= \sigma(W_{ij}Z_{ij} - U_{ij}V_{ij}),\\
\frac{W_{ij} - W_{i,j-1}}{\Delta y} &= \sigma(U_{ij}V_{ij} - W_{ij}Z_{ij}),\\
\frac{Z_{ij} - Z_{i,j+1}}{\Delta y} &= \sigma(U_{ij}V_{ij} - W_{ij}Z_{ij}).
\end{aligned}$$

Spatial discretization

Fixed-point iteration:

$$\sigma M_{ij}^{(k)} U_{ij}^{(k+1)} + \frac{U_{ij}^{(k+1)} - U_{i-1,j}^{(k+1)}}{\Delta x} = \sigma[W_{ij}^{(k)} Z_{ij}^{(k)} + (M_{ij}^{(k)} - V_{ij}^{(k)}) U_{ij}^{(k)}],$$

$$\sigma M_{ij}^{(k)} V_{ij}^{(k+1)} - \frac{V_{ij}^{(k+1)} - V_{i+1,j}^{(k+1)}}{\Delta x} = \sigma[W_{ij}^{(k)} Z_{ij}^{(k)} + (M_{ij}^{(k)} - U_{ij}^{(k)}) V_{ij}^{(k)}],$$

$$\sigma M_{ij}^{(k)} W_{ij}^{(k+1)} + \frac{W_{ij}^{(k+1)} - W_{i,j-1}^{(k+1)}}{\Delta y} = \sigma[U_{ij}^{(k)} V_{ij}^{(k)} + (M_{ij}^{(k)} - Z_{ij}^{(k)}) W_{ij}^{(k)}],$$

$$\sigma M_{ij}^{(k)} Z_{ij}^{(k+1)} - \frac{Z_{ij}^{(k+1)} - Z_{i,j+1}^{(k+1)}}{\Delta y} = \sigma[U_{ij}^{(k)} V_{ij}^{(k)} + (M_{ij}^{(k)} - W_{ij}^{(k)}) Z_{ij}^{(k)}].$$

Why is the convergence slow for large σ?

Add up the four equations and we have

$$\sigma M_{ij}^{(k)} M_{ij}^{(k+1)} + \cdots = \sigma M_{ij}^{(k)} M_{ij}^{(k)}$$

$$\Downarrow$$

$$M_{ij}^{(k+1)} = M_{ij}^{(k)} - \frac{1}{\sigma M_{ij}^{(k)}} (\cdots)$$

When σ is large, the change of M_{ij} is small.

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When σ is large, the change of M_{ij} is small.

We can also show that the update of $U_{ij} - V_{ij}$ and $W_{ij} - Z_{ij}$ is small when σ is large.

Why is the convergence slow for large σ?

In general, for any algebraic equations

$$\boldsymbol{T}(\boldsymbol{x}) = \frac{1}{\varepsilon}\boldsymbol{N}(\boldsymbol{x}),$$

the iterative method

$$\frac{\nu}{\varepsilon}\boldsymbol{x}^{(k+1)} + \boldsymbol{T}(\boldsymbol{x}^{(k+1)}) = \frac{1}{\varepsilon}(\boldsymbol{N}(\boldsymbol{x}^{(k)}) + \nu\boldsymbol{x}^{(k)})$$

may converge slowly for small ε if there exists a vector $\boldsymbol{\alpha}$ such that

$$\boldsymbol{\alpha}^T\boldsymbol{N}(\boldsymbol{x}) = 0, \qquad \forall \boldsymbol{x}.$$

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Symmetric Gauss-Seidel method

Idea: First update all the variables from left to right and from bottom to top, and then update them in reverse order.

Symmetric Gauss-Seidel method

Idea: First update all the variables from left to right and from bottom to top, and then update them in reverse order.

Left-to-right, bottom-to-top scan:

$$\frac{U_{ij}^{(k+1)} - U_{i-1,j}^{(k+1)}}{\Delta x} = \sigma(W_{ij}^{(k+1)} Z_{ij}^{(k+1)} - U_{ij}^{(k+1)} V_{ij}^{(k+1)}),$$

$$-\frac{V_{i+1,j}^{(k)} - V_{ij}^{(k+1)}}{\Delta x} = \sigma(W_{ij}^{(k+1)} Z_{ij}^{(k+1)} - U_{ij}^{(k+1)} V_{ij}^{(k+1)}),$$

$$\frac{W_{ij}^{(k+1)} - W_{i,j-1}^{(k+1)}}{\Delta y} = \sigma(U_{ij}^{(k+1)} V_{ij}^{(k+1)} - W_{ij}^{(k+1)} Z_{ij}^{(k+1)}),$$

$$-\frac{Z_{i,j+1}^{(k)} - Z_{ij}^{(k+1)}}{\Delta y} = \sigma(U_{ij}^{(k+1)} V_{ij}^{(k+1)} - W_{ij}^{(k+1)} Z_{ij}^{(k+1)}).$$

Symmetric Gauss-Seidel method

Idea: First update all the variables from left to right and from bottom to top, and then update them in reverse order.

Right-to-left, top-to-bottom scan:

$$\frac{U_{ij}^{(k+1)} - U_{i-1,j}^{(k)}}{\Delta x} = \sigma(W_{ij}^{(k+1)} Z_{ij}^{(k+1)} - U_{ij}^{(k+1)} V_{ij}^{(k+1)}),$$

$$-\frac{V_{i+1,j}^{(k+1)} - V_{ij}^{(k+1)}}{\Delta x} = \sigma(W_{ij}^{(k+1)} Z_{ij}^{(k+1)} - U_{ij}^{(k+1)} V_{ij}^{(k+1)}),$$

$$\frac{W_{ij}^{(k+1)} - W_{i,j-1}^{(k)}}{\Delta y} = \sigma(U_{ij}^{(k+1)} V_{ij}^{(k+1)} - W_{ij}^{(k+1)} Z_{ij}^{(k+1)}),$$

$$-\frac{Z_{i,j+1}^{(k+1)} - Z_{ij}^{(k+1)}}{\Delta y} = \sigma(U_{ij}^{(k+1)} V_{ij}^{(k+1)} - W_{ij}^{(k+1)} Z_{ij}^{(k+1)}).$$

Nonlinear equations

For each grid cell, we need to solve

$$\frac{1}{\Delta x}U_{ij} - \sigma(W_{ij}Z_{ij} - U_{ij}V_{ij}) = \frac{1}{\Delta x}U_{i-1,j},$$
$$\frac{1}{\Delta x}V_{ij} - \sigma(W_{ij}Z_{ij} - U_{ij}V_{ij}) = \frac{1}{\Delta x}V_{i+1,j},$$
$$\frac{1}{\Delta y}W_{ij} - \sigma(U_{ij}V_{ij} - W_{ij}Z_{ij}) = \frac{1}{\Delta y}W_{i,j-1},$$
$$\frac{1}{\Delta y}Z_{ij} - \sigma(U_{ij}V_{ij} - W_{ij}Z_{ij}) = \frac{1}{\Delta y}Z_{i,j+1}.$$

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$$\frac{1}{\Delta y}W_{ij} - \sigma(U_{ij}V_{ij} - W_{ij}Z_{ij}) = \frac{1}{\Delta y}W_{i,j-1},$$
$$\frac{1}{\Delta y}Z_{ij} - \sigma(U_{ij}V_{ij} - W_{ij}Z_{ij}) = \frac{1}{\Delta y}Z_{i,j+1}.$$

In order that the method can be generalized to the Boltzmann equation, we need an iterative solver for these quadratic equations.

Inner iterations

Let $M_{ij} = U_{ij} + V_{ij} + W_{ij} + Z_{ij}$.

Fixed-point iteration:

$$\left(\frac{1}{\Delta x} + \sigma M_{ij}^{(n)}\right) U_{ij}^{(n+1)} = \frac{1}{\Delta x} U_{i-1,j} + \sigma \left[W_{ij}^{(n)} Z_{ij}^{(n)} + (M_{ij}^{(n)} - V_{ij}^{(n)}) U_{ij}^{(n)}\right],$$

$$\left(\frac{1}{\Delta x} + \sigma M_{ij}^{(n)}\right) V_{ij}^{(n+1)} = \frac{1}{\Delta x} V_{i+1,j} + \sigma \left[W_{ij}^{(n)} Z_{ij}^{(n)} + (M_{ij}^{(n)} - U_{ij}^{(n)}) V_{ij}^{(n)}\right],$$

$$\left(\frac{1}{\Delta y} + \sigma M_{ij}^{(n)}\right) W_{ij}^{(n+1)} = \frac{1}{\Delta y} W_{i,j-1} + \sigma \left[U_{ij}^{(n)} V_{ij}^{(n)} + (M_{ij}^{(n)} - Z_{ij}^{(n)}) W_{ij}^{(n)}\right],$$

$$\left(\frac{1}{\Delta y} + \sigma M_{ij}^{(n)}\right) Z_{ij}^{(n+1)} = \frac{1}{\Delta y} Z_{i,j+1} + \sigma \left[U_{ij}^{(n)} V_{ij}^{(n)} + (M_{ij}^{(n)} - W_{ij}^{(n)}) Z_{ij}^{(n)}\right].$$

The update of M_{ij} is small when σ is large!

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An alternative form of the collision term

For $M = U + V + W + Z$, we have

$$\sigma(WZ - UV) = \sigma M \left(\frac{(U+W)(U+Z)}{U+V+W+Z} - U \right),$$

$$\sigma(WZ - UV) = \sigma M \left(\frac{(V+W)(V+Z)}{U+V+W+Z} - V \right),$$

$$\sigma(UV - WZ) = \sigma M \left(\frac{(W+U)(W+V)}{U+V+W+Z} - W \right),$$

$$\sigma(UV - WZ) = \sigma M \left(\frac{(Z+U)(Z+V)}{U+V+W+Z} - Z \right),$$

An alternative form of the collision term

For $M = U + V + W + Z$, we have

$$\begin{aligned}
\sigma(WZ - UV) &= \sigma M \left(U_\infty - U\right), \\
\sigma(WZ - UV) &= \sigma M \left(V_\infty - V\right), \\
\sigma(UV - WZ) &= \sigma M \left(W_\infty - W\right), \\
\sigma(UV - WZ) &= \sigma M \left(Z_\infty - Z\right),
\end{aligned}$$

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\sigma(UV - WZ) &= \sigma M (W_\infty - W), \\
\sigma(UV - WZ) &= \sigma M (Z_\infty - Z),
\end{aligned}$$

where

$$U_\infty = \frac{(U+W)(U+Z)}{U+V+W+Z}, \quad V_\infty = \frac{(V+W)(V+Z)}{U+V+W+Z},$$
$$W_\infty = \frac{(W+U)(W+V)}{U+V+W+Z}, \quad Z_\infty = \frac{(Z+U)(Z+V)}{U+V+W+Z}.$$

are the equilibrium values of U, V, W, and Z!

Equilibrium values

Let

$$M = U + V + W + Z, \quad P = U - V, \quad Q = W - Z.$$

Then

$$U_\infty = \frac{(U+W)(U+Z)}{U+V+W+Z} = \frac{(M+P+Q)(M+P-Q)}{4M},$$
$$V_\infty = \frac{(V+W)(V+Z)}{U+V+W+Z} = \frac{(M-P+Q)(M-P-Q)}{4M},$$
$$W_\infty = \frac{(W+U)(W+V)}{U+V+W+Z} = \frac{(M+P+Q)(M-P+Q)}{4M},$$
$$Z_\infty = \frac{(Z+U)(Z+V)}{U+V+W+Z} = \frac{(M+P-Q)(M-P-Q)}{4M}.$$

Nonlinear equations

We want to solve

$$\begin{aligned}
\frac{1}{\Delta x}U_{ij} - \sigma M_{ij}(U_{\infty,ij} - U_{ij}) &= \frac{1}{\Delta x}U_{i-1,j}, \\
\frac{1}{\Delta x}V_{ij} - \sigma M_{ij}(V_{\infty,ij} - V_{ij}) &= \frac{1}{\Delta x}V_{i+1,j}, \\
\frac{1}{\Delta y}W_{ij} - \sigma M_{ij}(W_{\infty,ij} - W_{ij}) &= \frac{1}{\Delta y}W_{i,j-1}, \\
\frac{1}{\Delta y}Z_{ij} - \sigma M_{ij}(Z_{\infty,ij} - Z_{ij}) &= \frac{1}{\Delta y}Z_{i,j+1}.
\end{aligned}$$

For the fixed-point iteration, the update of

$$M_{ij} = U_{ij}+V_{ij}+W_{ij}+Z_{ij}, \quad P_{ij} = U_{ij}-V_{ij}, \quad Q_{ij} = W_{ij}-Z_{ij}$$

is small when σ is large.

Can we solve M_{ij}, P_{ij}, and Q_{ij} directly?

By taking the difference of the first two equations

$$\frac{1}{\Delta x}U_{ij} - \sigma M_{ij}(U_{\infty,ij} - U_{ij}) = \frac{1}{\Delta x}U_{i-1,j},$$
$$\frac{1}{\Delta x}V_{ij} - \sigma M_{ij}(V_{\infty,ij} - V_{ij}) = \frac{1}{\Delta x}V_{i+1,j},$$

we get

$$P_{ij} = U_{ij} - V_{ij} = U_{i-1,j} - V_{i+1,j}.$$

Similarly,

$$Q_{ij} = W_{ij} - Z_{ij} = W_{i,j-1} - Z_{i,j+1}.$$

Can we solve M_{ij}, P_{ij}, and Q_{ij} directly?

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we get

$$P_{ij} = U_{ij} - V_{ij} = U_{i-1,j} - V_{i+1,j}.$$

Similarly,

$$Q_{ij} = W_{ij} - Z_{ij} = W_{i,j-1} - Z_{i,j+1}.$$

However, we cannot solve M_{ij} directly.

Approximation of M_{ij}

Adding up the four equations yields

$$\frac{U_{ij}+V_{ij}}{\Delta x}+\frac{W_{ij}+Z_{ij}}{\Delta y}=\frac{U_{i-1,j}+V_{i+1,j}}{\Delta x}+\frac{W_{i,j-1}+Z_{i,j+1}}{\Delta y}.$$

For large σ, we perform the following split:

$$U_{ij}=\underbrace{U_{\infty,ij}}_{\text{large}}+\underbrace{\delta U_{ij}}_{\text{small}},\quad V_{ij}=\underbrace{V_{\infty,ij}}_{\text{large}}+\underbrace{\delta V_{ij}}_{\text{small}},$$

$$W_{ij}=\underbrace{W_{\infty,ij}}_{\text{large}}+\underbrace{\delta W_{ij}}_{\text{small}},\quad Z_{ij}=\underbrace{Z_{\infty,ij}}_{\text{large}}+\underbrace{\delta Z_{ij}}_{\text{small}}.$$

Approximation of M_{ij}

$$\frac{U_{\infty,ij} + V_{\infty,ij}}{\Delta x} + \frac{W_{\infty,ij} + Z_{\infty,ij}}{\Delta y} = C_{ij},$$

Approximation of M_{ij}

$$\frac{U_{\infty,ij} + V_{\infty,ij}}{\Delta x} + \frac{W_{\infty,ij} + Z_{\infty,ij}}{\Delta y} = C_{ij},$$

where

$$\begin{aligned} C_{ij} &= \frac{U_{i-1,j} + V_{i+1,j}}{\Delta x} + \frac{W_{i,j-1} + Z_{i,j+1}}{\Delta y} \\ &\quad - \frac{\delta U_{ij} + \delta V_{ij}}{\Delta x} - \frac{\delta W_{ij} + \delta Z_{ij}}{\Delta y} \\ &= \frac{U_{i-1,j} + V_{i+1,j}}{\Delta x} + \frac{W_{i,j-1} + Z_{i,j+1}}{\Delta y} \\ &\quad - \frac{2(U_{ij}V_{ij} - W_{ij}Z_{ij})}{U_{ij} + V_{ij} + W_{ij} + Z_{ij}} \left(\frac{1}{\Delta x} - \frac{1}{\Delta y} \right). \end{aligned}$$

Approximation of M_{ij}

1. Use the current solution to approximate C_{ij} ($C_{ij} \approx C_{ij}^{(n)}$).
2. Solve M_{ij} from the equation

$$\frac{U_{\infty,ij} + V_{\infty,ij}}{\Delta x} + \frac{W_{\infty,ij} + Z_{\infty,ij}}{\Delta y} = C_{ij}^{(n)}.$$

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1. Use the current solution to approximate C_{ij} ($C_{ij} \approx C_{ij}^{(n)}$).
2. Solve M_{ij} from the equation

$$\frac{U_{\infty,ij} + V_{\infty,ij}}{\Delta x} + \frac{W_{\infty,ij} + Z_{\infty,ij}}{\Delta y} = C_{ij}^{(n)}.$$

Summary:

$$P_{ij}^{(*)} = U_{i-1,j} - V_{i+1,j}, \quad Q_{ij}^{(*)} = W_{i,j-1} - Z_{i,j+1},$$

$$M_{ij}^{(*)} = \left(\frac{1}{\Delta x} + \frac{1}{\Delta y}\right)^{-1} \times$$

$$\left[C_{ij}^{(n)} + \sqrt{(C_{ij}^{(n)})^2 - \left[\left(P_{ij}^{(*)}\right)^2 - \left(Q_{ij}^{(*)}\right)^2\right]\left(\frac{1}{\Delta x^2} - \frac{1}{\Delta y^2}\right)}\right].$$

Inner iterations

We would like to solve

$$\begin{aligned}
\frac{1}{\Delta x}U_{ij} - \sigma M_{ij}(U_{\infty,ij} - U_{ij}) &= \frac{1}{\Delta x}U_{i-1,j}, \\
\frac{1}{\Delta x}V_{ij} - \sigma M_{ij}(V_{\infty,ij} - V_{ij}) &= \frac{1}{\Delta x}V_{i+1,j}, \\
\frac{1}{\Delta y}W_{ij} - \sigma M_{ij}(W_{\infty,ij} - W_{ij}) &= \frac{1}{\Delta y}W_{i,j-1}, \\
\frac{1}{\Delta y}Z_{ij} - \sigma M_{ij}(Z_{\infty,ij} - Z_{ij}) &= \frac{1}{\Delta y}Z_{i,j+1}.
\end{aligned}$$

General procedure:

$$\begin{aligned}
U_{ij}^{(n)}, V_{ij}^{(n)}, W_{ij}^{(n)}, Z_{ij}^{(n)} &\to P_{ij}^{(*)}, Q_{ij}^{(*)}, M_{ij}^{(*)} \\
&\to U_{\infty,ij}^{(*)}, V_{\infty,ij}^{(*)}, W_{\infty,ij}^{(*)}, Z_{\infty,ij}^{(*)} \\
&\to U_{ij}^{(n+1)}, V_{ij}^{(n+1)}, W_{ij}^{(n+1)}, Z_{ij}^{(n+1)}.
\end{aligned}$$

1 Fixed-point iteration for the Broadwell model

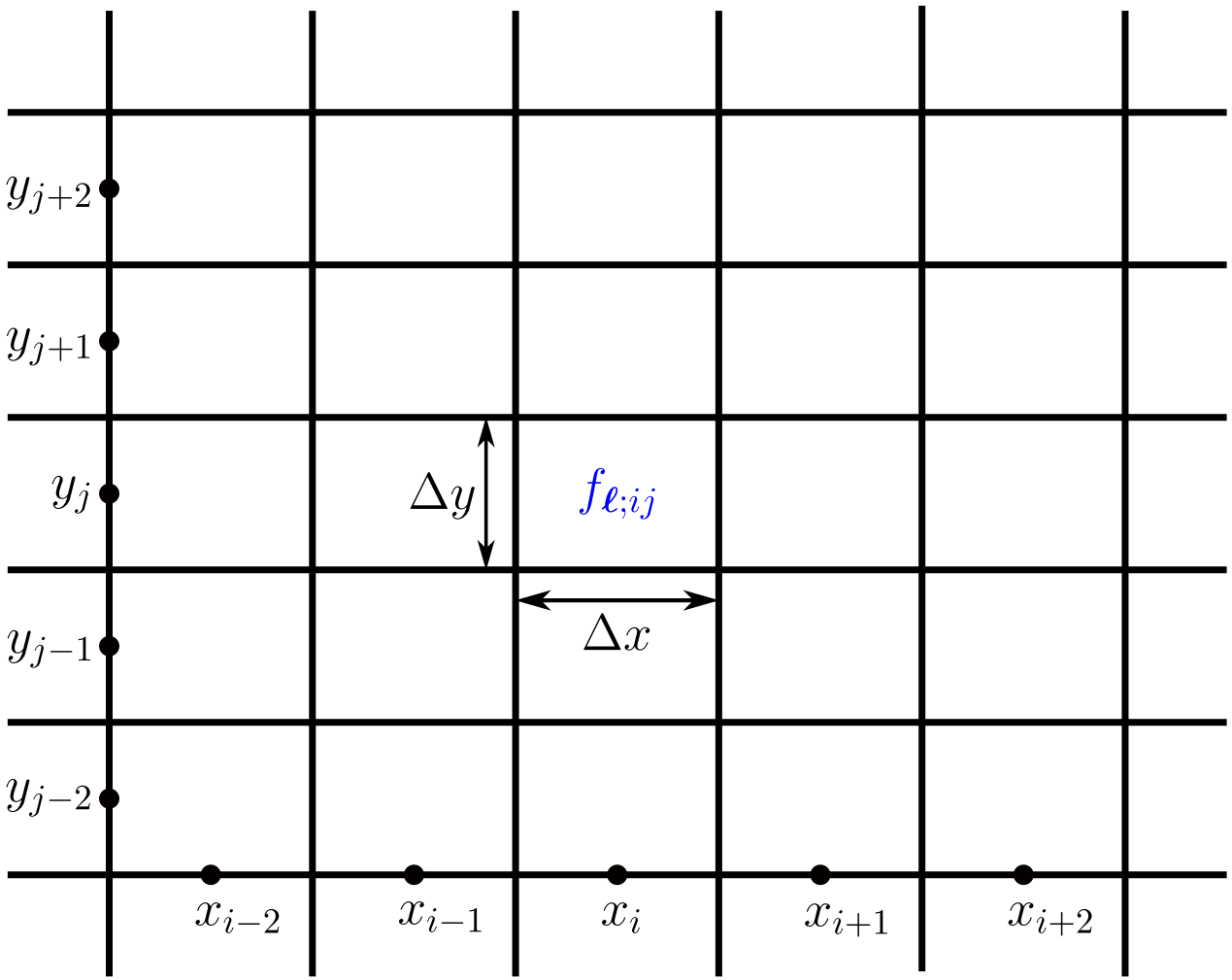
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Discretization of the distribution function



Steady-state Boltzmann equation

Two-dimensional steady-state Boltzmann equation:

$$v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \frac{1}{\varepsilon} Q(f, f).$$

Steady-state Boltzmann equation

Two-dimensional steady-state Boltzmann equation:

$$v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \frac{1}{\varepsilon} Q(f, f).$$

Upwind method: $v_{\boldsymbol{\ell}} = \boldsymbol{\ell} L/N,$

$$v_{x,\boldsymbol{\ell}}^{+} \frac{f_{\boldsymbol{\ell};ij} - f_{\boldsymbol{\ell};i-1,j}}{\Delta x} + v_{x,\boldsymbol{\ell}}^{-} \frac{f_{\boldsymbol{\ell};i+1,j} - f_{\boldsymbol{\ell};ij}}{\Delta x}$$
$$+ v_{y,\boldsymbol{\ell}}^{+} \frac{f_{\boldsymbol{\ell};ij} - f_{\boldsymbol{\ell};i,j-1}}{\Delta y} + v_{y,\boldsymbol{\ell}}^{-} \frac{f_{\boldsymbol{\ell};i,j+1} - f_{\boldsymbol{\ell};ij}}{\Delta y} = \frac{1}{\varepsilon} Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}, \boldsymbol{f}_{ij}).$$

Steady-state Boltzmann equation

Two-dimensional steady-state Boltzmann equation:

$$v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} = \frac{1}{\varepsilon} Q(f, f).$$

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$$v_{x,\boldsymbol{\ell}}^{+} \frac{f_{\boldsymbol{\ell};ij} - f_{\boldsymbol{\ell};i-1,j}}{\Delta x} + v_{x,\boldsymbol{\ell}}^{-} \frac{f_{\boldsymbol{\ell};i+1,j} - f_{\boldsymbol{\ell};ij}}{\Delta x} + v_{y,\boldsymbol{\ell}}^{+} \frac{f_{\boldsymbol{\ell};ij} - f_{\boldsymbol{\ell};i,j-1}}{\Delta y} + v_{y,\boldsymbol{\ell}}^{-} \frac{f_{\boldsymbol{\ell};i,j+1} - f_{\boldsymbol{\ell};ij}}{\Delta y} = \frac{1}{\varepsilon} Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}, \boldsymbol{f}_{ij}).$$

Can you write down the symmetric Gauss-Seidel method for this equation?

Inner iterations

Nonlinear equations: For each grid cell, we need to solve

$$\left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x}+\frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y}\right) f_{\boldsymbol{\ell};ij}=\frac{1}{\varepsilon}Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij},\boldsymbol{f}_{ij})+g_{\boldsymbol{\ell},ij},$$

where $g_{\boldsymbol{\ell},ij}$ is a known function.

- For the fixed-point iteration, The density ρ_{ij}, momentum $\boldsymbol{m}_{ij}$, and energy E_{ij} are updated slowly when ε is small.
- Accelerated iterative method:

$$\boldsymbol{f}_{ij}^{(n)}\to\mathcal{M}_{ij}^{(*)}\to\boldsymbol{f}_{ij}^{(n+1)}.$$

Step 1: $\boldsymbol{f}_{ij}^{(n)} \to \mathcal{M}_{ij}^{(*)}$

Let

$$\boldsymbol{\varphi}(\boldsymbol{v}) = \begin{pmatrix} 1 \\ \boldsymbol{v} \\ |\boldsymbol{v}|^2 \end{pmatrix}.$$

Then

$$\left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y} \right) f_{\boldsymbol{\ell};ij} = \frac{1}{\varepsilon} Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}, \boldsymbol{f}_{ij}) + g_{\boldsymbol{\ell},ij}$$

$$\Downarrow$$

$$\sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) \left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y} \right) f_{\boldsymbol{\ell};ij} = \sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) g_{\boldsymbol{\ell},ij}$$

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$$\Downarrow$$

$$\sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) \left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y} \right) [\mathcal{M}_{\boldsymbol{\ell};ij} + (f_{\boldsymbol{\ell};ij} - \mathcal{M}_{\boldsymbol{\ell};ij})] = \sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) g_{\boldsymbol{\ell},ij}$$

Step 1: $\boldsymbol{f}_{ij}^{(n)} \to \mathcal{M}_{ij}^{(*)}$

Let

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Then

$$\left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y} \right) f_{\boldsymbol{\ell};ij} = \frac{1}{\varepsilon} Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}, \boldsymbol{f}_{ij}) + g_{\boldsymbol{\ell},ij}$$

$$\Downarrow$$

$$\sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) \left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y} \right) [\mathcal{M}_{\boldsymbol{\ell};ij}^{(*)} + (f_{\boldsymbol{\ell};ij}^{(n)} - \mathcal{M}_{\boldsymbol{\ell};ij}^{(n)})] = \sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) g_{\boldsymbol{\ell},ij}$$

Step 1: $\boldsymbol{f}_{ij}^{(n)} \to \mathcal{M}_{ij}^{(*)}$

Recall that

$$\mathcal{M}_{\boldsymbol{\ell};ij}^{(*)} = \exp\left(\alpha_{ij}^{(*)} + \boldsymbol{\beta}_{ij}^{(*)} \cdot \boldsymbol{v}_{\boldsymbol{\ell}} + \gamma_{ij}^{(*)} |\boldsymbol{v}_{\boldsymbol{\ell}}|^2\right).$$

We can solve $\alpha_{ij}^{(*)}$, $\boldsymbol{\beta}_{ij}^{(*)}$, and $\gamma_{ij}^{(*)}$ by Newton's method from

$$\sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) \left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y}\right) [\mathcal{M}_{\boldsymbol{\ell};ij}^{(*)} + (f_{\boldsymbol{\ell};ij}^{(n)} - \mathcal{M}_{\boldsymbol{\ell};ij}^{(n)})] = \sum_{\boldsymbol{\ell}} \boldsymbol{\varphi}(\boldsymbol{v}_{\boldsymbol{\ell}}) g_{\boldsymbol{\ell},ij}.$$

Step 2: $\mathcal{M}_{ij}^{(*)} \to \boldsymbol{f}_{ij}^{(n+1)}$

Fixed-point iteration:

$$\left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x} + \frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y} + \frac{1}{\varepsilon} \nu_{\boldsymbol{\ell};ij}^{(n)} \right) f_{\boldsymbol{\ell};ij}^{(n+1)} = \frac{1}{\varepsilon} Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}^{(n)}, \boldsymbol{f}_{ij}^{(n)}) + g_{\boldsymbol{\ell},ij} + \frac{1}{\varepsilon} \nu_{\boldsymbol{\ell};ij}^{(n)} f_{\boldsymbol{\ell};ij}^{(n)}.$$

Step 2: $\mathcal{M}_{ij}^{(*)} \to \boldsymbol{f}_{ij}^{(n+1)}$

Fixed-point iteration:

$$\left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x}+\frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y}+\frac{1}{\varepsilon}\nu_{\boldsymbol{\ell};ij}^{(n)}\right) f_{\boldsymbol{\ell};ij}^{(n+1)} = \frac{1}{\varepsilon}Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}^{(n)},\boldsymbol{f}_{ij}^{(n)})+g_{\boldsymbol{\ell},ij}+\frac{1}{\varepsilon}\nu_{\boldsymbol{\ell};ij}^{(n)}f_{\boldsymbol{\ell};ij}^{(n)}.$$

Improved iteration:

$$\left(\frac{|v_{x,\boldsymbol{\ell}}|}{\Delta x}+\frac{|v_{y,\boldsymbol{\ell}}|}{\Delta y}+\frac{1}{\varepsilon}\nu_{\boldsymbol{\ell};ij}^{(n)}\right) f_{\boldsymbol{\ell};ij}^{(n+1)} = \frac{1}{\varepsilon}Q_{\boldsymbol{\ell}}(\boldsymbol{f}_{ij}^{(n)},\boldsymbol{f}_{ij}^{(n)})+g_{\boldsymbol{\ell},ij}+\frac{1}{\varepsilon}\nu_{\boldsymbol{\ell};ij}^{(n)}(f_{\boldsymbol{\ell};ij}^{(n)}-\mathcal{M}_{\boldsymbol{\ell};ij}^{(n)}+\mathcal{M}_{\boldsymbol{\ell};ij}^{(*)}).$$

1 Fixed-point iteration for the Broadwell model

2 Symmetric Gauss-Seidel Method for the Broadwell equation

3 Acceleration of inner iterations

4 Symmetric Gauss-Seidel method for the Boltzmann equation

5 Summary

Summary

Iterative methods for the Broadwell model:

- Fixed-point iteration – slow convergence for large σ
- Symmetric Gauss-Seidel method
- Accelerated inner iterations

Iterative methods for the Boltzmann equation:

- Symmetric Gauss-Seidel method
- Accelerated inner iterations