Transported Probability Density Function (PDF) Methods for Multiscale and Uncertainty Problems - Part II

A Solution Algorithm for the Fluid Dynamic Equations Based on a Stochastic Model for Molecular Motion

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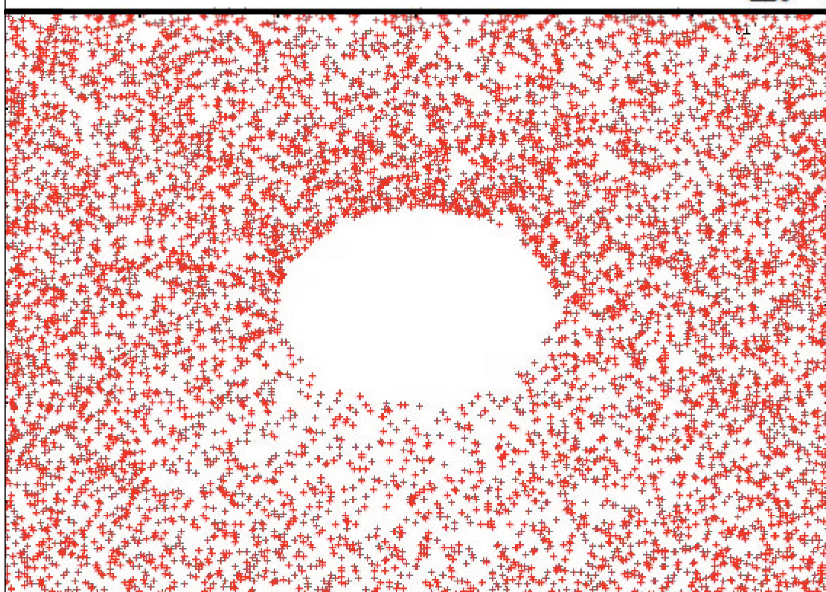
Fokker Planck Equation for PDF Evolution

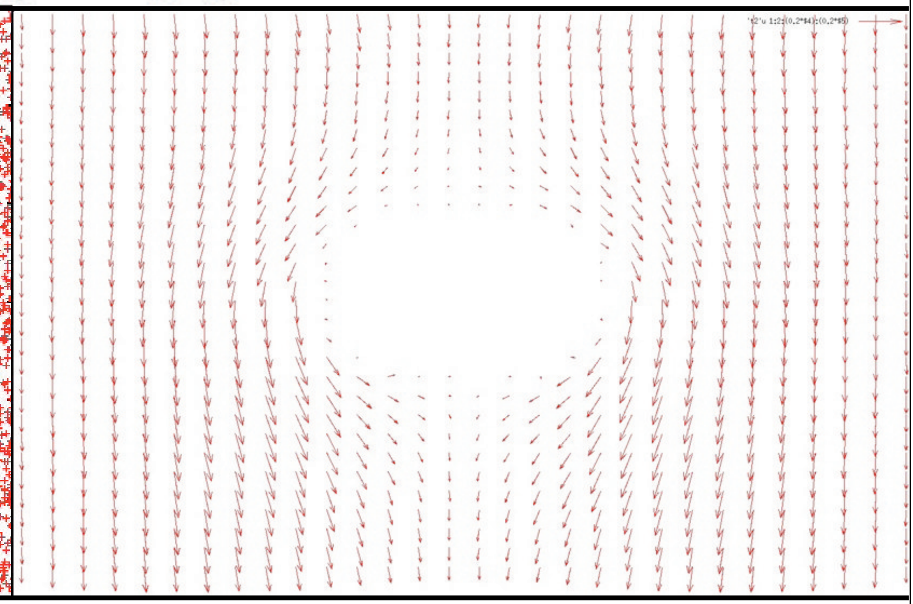
$$\frac{\partial f_{\boldsymbol{X}}(\boldsymbol{x};t)}{\partial t} = -\frac{\partial D_i^{(1)} f_{\boldsymbol{X}}(\boldsymbol{x};t)}{\partial x_i} + \frac{\partial^2 D_{ij}^{(2)} f_{\boldsymbol{X}}(\boldsymbol{x};t)}{\partial x_i \partial x_j}$$

with with

$$D_i^{(1)} = \lim_{\Delta t \to 0} \frac{\langle \Delta X_i | \boldsymbol{x}; t \rangle}{\Delta t}$$

$$D_{ij}^{(2)} = \lim_{\Delta t \to 0} \frac{\langle \Delta X_i \Delta X_j | \boldsymbol{x}; t \rangle}{2\Delta t}.$$

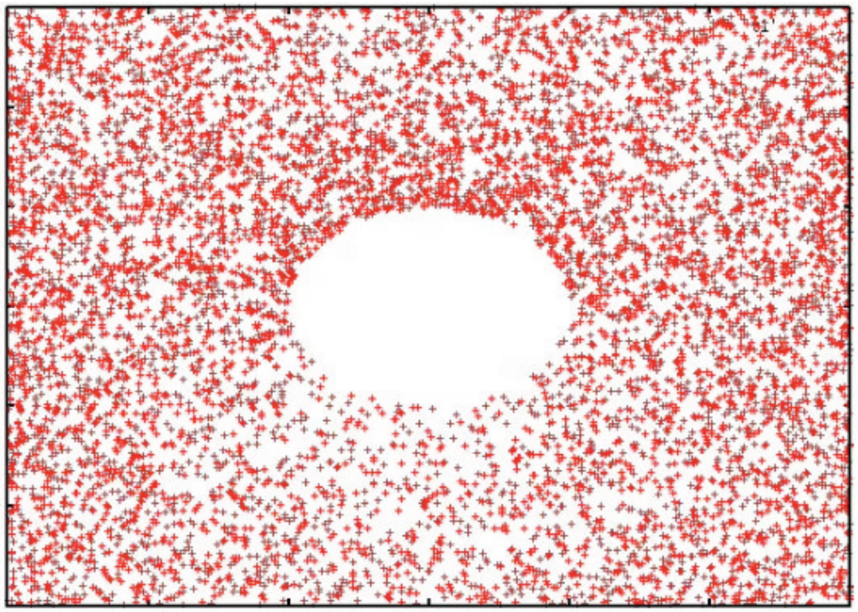




Outline

- Kinetic Description of Non-Equilibrium Gas
- Consistency with Continuum Fluid Dynamics
- Collision Models
- Fokker Planck Model and Integration Scheme
- Knudsen Paradox
- Performance
- Conclusion

Kinetic Description of Non-Equilibrium Gas



Assume that the statistics of particles in a monatomic gas can be described by the mass density function

$$\mathcal{F}(\boldsymbol{V},\boldsymbol{x},t) = \rho(\boldsymbol{x},t) f(\boldsymbol{V};\boldsymbol{x},t)$$

$$\frac{\partial \mathcal{F}}{\partial t} + V_i \frac{\partial \mathcal{F}}{\partial x_i} + \frac{\partial F_i \mathcal{F}}{\partial V_i} = S(\mathcal{F})$$

In equilibrium, the velocity PDF is given by the Maxwell distribution:

$$\left(\rho, \rho\boldsymbol{U}, \rho e_s + \tfrac{1}{2}\rho\boldsymbol{U}^2\right) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$$ with the weights $$\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \tfrac{1}{2}\boldsymbol{V}^2\right)$$

Consistency with Fluid Dynamics

$(\rho, \rho \boldsymbol{U}, \rho e_s + \frac{1}{2}\rho \boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$ with the weights $\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \frac{1}{2}\boldsymbol{V}^2\right)$

transfer equations for $\boldsymbol{\Psi}_{\text{cons}}$ yield the conservation laws

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0,$$

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} + \frac{\partial p_{ij}}{\partial x_j} = \rho F_i,$$

$$\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk}\frac{\partial U_j}{\partial x_k} = 0.$$

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do not depend on the details of the collision model due to conservation property

$$\int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} S(\mathcal{F}) d\boldsymbol{V} = 0 \quad \text{for any} \quad \mathcal{F}$$

Consistency with Fluid Dynamics

$(\rho, \rho \boldsymbol{U}, \rho e_s + \frac{1}{2}\rho \boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$ with the weights $\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \frac{1}{2}\boldsymbol{V}^2\right)$

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$$\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk}\frac{\partial U_j}{\partial x_k} = 0.$$

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unknown molecular stress p_{ij}

splitting $p_{ij} = p\delta_{ij} + \pi_{ij}$ $\qquad p = \frac{2}{3}\rho e_s$

For perfect gases we are familiar with the equation of state $p = (\gamma - 1)\rho e_s$

$\gamma = 5/3$

Consistency with Fluid Dynamics

$(\rho, \rho\boldsymbol{U}, \rho e_s + \frac{1}{2}\rho\boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$ with the weights $\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \frac{1}{2}\boldsymbol{V}^2\right)$

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$$\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk}\frac{\partial U_j}{\partial x_k} = 0.$$

$$\frac{\partial \pi_{ij}}{\partial t} + \frac{\partial \pi_{ij} U_k}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2p\frac{\partial U_{\langle i}}{\partial x_{j\rangle}} + 2\pi_{k\langle i}\frac{\partial U_{j\rangle}}{\partial x_k} = P_{ij}$$

$$\frac{\partial q_i}{\partial t} + \frac{\partial q_i U_k}{\partial x_k} + \frac{1}{2}\frac{\partial R_{ik}}{\partial x_k} + p\frac{\partial(\pi_{ik}/\rho)}{\partial x_k} + \frac{5}{2}\frac{k}{m}p_{ik}\frac{\partial T}{\partial x_k} - \frac{\pi_{ij}}{\varrho}\frac{\partial \pi_{jk}}{\partial x_k} + \left(m_{ijk} + \frac{6}{5}q_{(i}\delta_{jk)} + q_k\delta_{ij}\right)\frac{\partial U_j}{\partial x_k} = P_i$$

collision model enters through P_{ij} and P_i

closure for the deviatoric stress π_{ij} and the heat flux q_i

Consistency with Fluid Dynamics

$$(\rho, \rho \boldsymbol{U}, \rho e_s + \tfrac{1}{2}\rho \boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$$ with the weights $\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \tfrac{1}{2}\boldsymbol{V}^2\right)$

transfer equations for $\boldsymbol{\Psi}_{\text{cons}}$ yield the conservation laws

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} &= 0, \\
\frac{\partial \rho U_i}{\partial t} + \frac{\partial \rho U_i U_j}{\partial x_j} + \frac{\partial p_{ij}}{\partial x_j} &= \rho F_i, \\
\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk} \frac{\partial U_j}{\partial x_k} &= 0.
\end{aligned}$$

Chapman-Enskog Expansion => Navier-Stokes

$$\pi_{ij} = -2\hat{\tau} p\, S^d_{ij} + \mathcal{O}\left(\tau^2\right) \quad \text{and}$$

$$q_i = -\frac{5}{2}\lambda \frac{k}{m}\hat{\tau} p \frac{\partial T}{\partial x_i} + \mathcal{O}\left(\tau^2\right)$$

with $S^d_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{1}{3}\frac{\partial U_n}{\partial x_n}\delta_{ij}$

Collision Models

$(\rho, \rho \boldsymbol{U}, \rho e_s + \frac{1}{2}\rho \boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\rm cons} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\rm cons} \mathcal{F}_M d\boldsymbol{V}$ with the weights $\boldsymbol{\Psi}_{\rm cons} = \left(1, \boldsymbol{V}, \frac{1}{2}\boldsymbol{V}^2\right)$

transfer equations for $\boldsymbol{\Psi}_{\rm cons}$ yield the conservation laws

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} = 0,$$
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$$\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk}\frac{\partial U_j}{\partial x_k} = 0.$$

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if $S^{(\rm Boltz)}$ is the benchmark, it is also reasonable to aim for

$$\int_{\mathbb{R}^3} \boldsymbol{\Psi} S(\mathcal{F}) d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi} S^{(\rm Boltz)}(\mathcal{F}) d\boldsymbol{V}$$

for integration weights $\boldsymbol{\Psi} = (V_i V_j, V_i V_j V_k, ..., V_{i_1} V_{i_2} \cdots V_{i_N})$

Collision Models

$(\rho, \rho \boldsymbol{U}, \rho e_s + \frac{1}{2}\rho \boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$ with the weights $\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \frac{1}{2}\boldsymbol{V}^2\right)$

transfer equations for $\boldsymbol{\Psi}_{\text{cons}}$ yield the conservation laws

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\frac{\partial \rho}{\partial t} + \frac{\partial \rho U_j}{\partial x_j} &= 0, \\
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\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk}\frac{\partial U_j}{\partial x_k} &= 0.
\end{aligned}$$

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most popular collision model is the so-called BGK model

$$S^{(\text{BGK})}(\mathcal{F}) = \frac{1}{\tau_{\text{BGK}}}\left(\mathcal{F}_M - \mathcal{F}\right)$$

assuming that the post-collision velocities follow a Maxwell

Collision Models

$(\rho, \rho \boldsymbol{U}, \rho e_s + \frac{1}{2}\rho \boldsymbol{U}^2) = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F} d\boldsymbol{V} = \int_{\mathbb{R}^3} \boldsymbol{\Psi}_{\text{cons}} \mathcal{F}_M d\boldsymbol{V}$ with the weights $\boldsymbol{\Psi}_{\text{cons}} = \left(1, \boldsymbol{V}, \frac{1}{2}\boldsymbol{V}^2\right)$

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$$\frac{\partial \rho e_s}{\partial t} + \frac{\partial \rho U_j e_s}{\partial x_j} + \frac{\partial q_j}{\partial x_j} + p_{jk}\frac{\partial U_j}{\partial x_k} = 0.$$

Here we propose a Fokker-Planck operator:

$$S^{(\text{FP})}(\mathcal{F}) = \frac{\partial}{\partial V_i}\left(\frac{1}{\tau_{\text{FP}}}(V_i - U_i)\mathcal{F}\right) + \frac{\partial^2}{\partial V_k \partial V_k}\left(\frac{2e_s}{3\tau_{\text{FP}}}\mathcal{F}\right)$$

depending explicitly on gas velocity $\boldsymbol{U}$, energy e_s and a relaxation time τ_{FP}

motivation: leads to the possibility to use highly efficient numerical methods

Collision Models

$$P_{ij}^{(\mathrm{Boltz})} = -\alpha \tfrac{\rho}{m} p_{\langle ij \rangle} \qquad P_i^{(\mathrm{Boltz})} = -\frac{2}{3}\alpha \frac{\rho}{m} q_i$$

$$P_{ij}^{(\mathrm{BGK})} = -\frac{1}{\tau_{\mathrm{BGK}}} p_{\langle ij \rangle} \quad P_i^{(\mathrm{BGK})} = -\frac{1}{\tau_{\mathrm{BGK}}} q_i$$

$$P_{ij}^{(\mathrm{FP})} = -\frac{2}{\tau_{\mathrm{FP}}} p_{\langle ij \rangle} \qquad P_i^{(\mathrm{FP})} = -\frac{3}{\tau_{\mathrm{FP}}} q_i,$$

$$\mathrm{Pr}^{(\mathrm{Boltz})} = \frac{2}{3}, \quad \mathrm{Pr}^{(\mathrm{BGK})} = 1 \quad \text{and} \quad \mathrm{Pr}^{(\mathrm{FP})} = \frac{3}{2}$$

All models are linear in the pressure deviator $p_{\langle ij \rangle}$ and the heat flux q_i

$$\frac{\partial \pi_{ij}}{\partial t} + \frac{\partial \pi_{ij} U_k}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2p \frac{\partial U_{\langle i}}{\partial x_{j\rangle}} + 2\pi_{k\langle i} \frac{\partial U_{j\rangle}}{\partial x_k} = P_{ij}$$

$$\frac{\partial q_i}{\partial t} + \frac{\partial q_i U_k}{\partial x_k} + \frac{1}{2}\frac{\partial R_{ik}}{\partial x_k} + p \frac{\partial (\pi_{ik}/\rho)}{\partial x_k} + \frac{5}{2}\frac{k}{m} p_{ik} \frac{\partial T}{\partial x_k} - \frac{\pi_{ij}}{\varrho}\frac{\partial \pi_{jk}}{\partial x_k} + \left(m_{ijk} + \frac{6}{5} q_{(i}\delta_{jk)} + q_k \delta_{ij}\right)\frac{\partial U_j}{\partial x_k} = P_i$$

collision model enters through P_{ij} and P_i

closure for the deviatoric stress π_{ij} and the heat flux q_i

Fokker-Planck Solution Algorithm

$$\frac{\partial \mathcal{F}}{\partial t} + V_i \frac{\partial \mathcal{F}}{\partial x_i} + \frac{\partial F_i \mathcal{F}}{\partial V_i} = S^{(\mathrm{FP})}(\mathcal{F}) = \frac{\partial}{\partial V_i}\left(\frac{1}{\tau_{\mathrm{FP}}}(V_i - U_i)\mathcal{F}\right) + \frac{\partial^2}{\partial V_k \partial V_k}\left(\frac{2e_s}{3\tau_{\mathrm{FP}}}\mathcal{F}\right)$$

Fokker-Planck equation $\frac{\partial \mathcal{F}}{\partial t} + V_i \frac{\partial \mathcal{F}}{\partial x_i} + \frac{\partial}{\partial V_i}\left\{\left[F_i - \frac{1}{\tau}(V_i - U_i)\right]\mathcal{F}\right\} = \frac{\partial^2}{\partial V_i \partial V_i}\left\{\frac{2e_s}{3\tau}\mathcal{F}\right\}$

solved through stochastic motion of notional particles

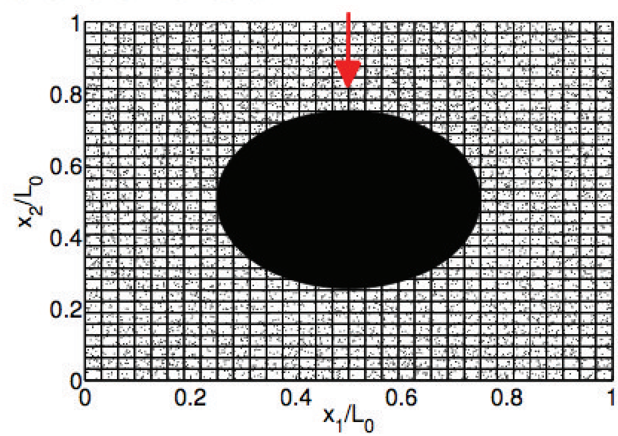
$$\frac{dX_i}{dt} = M_i \quad \text{with}$$

$$\frac{dM_i}{dt} = -\frac{1}{\tau}(M_i - U_i) + \left(\frac{4e_s}{3\tau}\right)^{1/2} \frac{dW_i(t)}{dt} + F_i$$

Fokker-Planck Solution Algorithm

n_t time steps are performed

(1) $\boldsymbol{U}$ and e_s at time t are estimated at each grid node and interpolated to the particle positions,
(2) the time step size Δt is determined,
(3) a first half-step is performed to estimate the particle mid-points,
(4) mid-point boundary conditions are applied,
(5) $\boldsymbol{U}$ and e_s at time $t + \Delta t/2$ are interpolated from the grid nodes to the particle mid-point positions,
(6) the new particle velocities and positions are computed, and
(7) the boundary conditions are enforced.



in statistical steady state $\boldsymbol{U}$ and e_s do not depend on the time.