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

A Solution Algorithm for the Fluid Dynamic Equations Based on a Stochastic Model for Molecular Motion (cont.)

Patrick Jenny (IFD, ETH Zürich)

Manuel Torrilhon (SAM, ETH Zürich)

Stefan Heinz (Dept. of Mathematics, University of Wyoming)

Fokker-Planck Solution Algorithm

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

solved through stochastic motion of notional particles

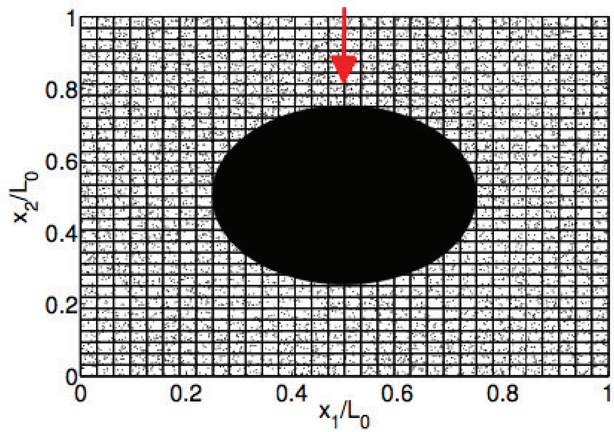
$$\frac{dX_i}{dt} = M_i \quad \text{with}$$

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

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.



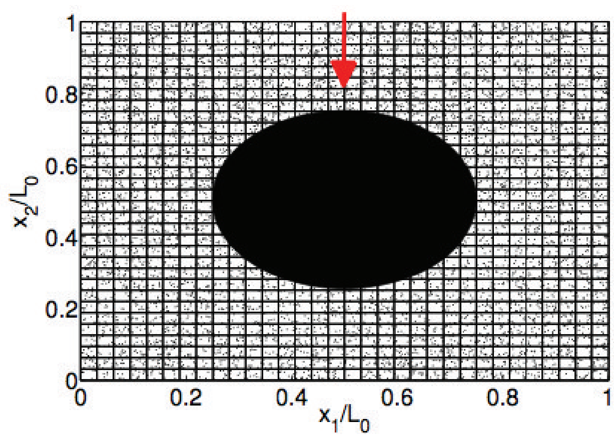
in statistical steady state $\boldsymbol{U}$ and e_s do not depend on the time.

Estimation of Statistical Moments

$$\mathcal{U}^J(t) = \sum_{j=1}^{N_p} \left\{ \hat{g}^J(\boldsymbol{X}^j(t)) \boldsymbol{M}^j(t) \right\},$$

$$\mathcal{E}^J(t) = \sum_{j=1}^{N_p} \left\{ \hat{g}^J(\boldsymbol{X}^j(t)) \boldsymbol{M}^j(t) \cdot \boldsymbol{M}^j(t) \right\}$$

$$\mathcal{W}^J(t) = \sum_{j=1}^{N_p} \left\{ \hat{g}^J(\boldsymbol{X}^j(t)) \right\},$$



$$\boldsymbol{U}(\boldsymbol{x}^J, t) = \frac{\mathcal{U}^J(t)}{\mathcal{W}^J(t)}$$

$$\boldsymbol{e}_s(\boldsymbol{x}^J, t) = \frac{1}{2} \left(\frac{\mathcal{E}^J(t)}{\mathcal{W}^J(t)} - \boldsymbol{U}^J(t) \cdot \boldsymbol{U}^J(t) \right)$$

Estimation of Statistical Moments

$$\mathcal{U}^J(t) = \mu\mathcal{U}^J(t-\Delta t) + (1-\mu)\sum_{j=1}^{N_p}\left\{\hat{g}^J(\boldsymbol{X}^j(t))\boldsymbol{M}^j(t)\right\},$$

$$\mathcal{E}^J(t) = \mu\mathcal{E}^J(t-\Delta t) + (1-\mu)\sum_{j=1}^{N_p}\left\{\hat{g}^J(\boldsymbol{X}^j(t))\boldsymbol{M}^j(t)\cdot\boldsymbol{M}^j(t)\right\}$$

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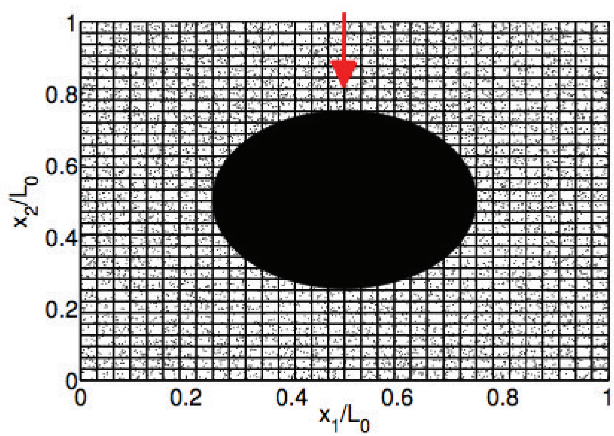


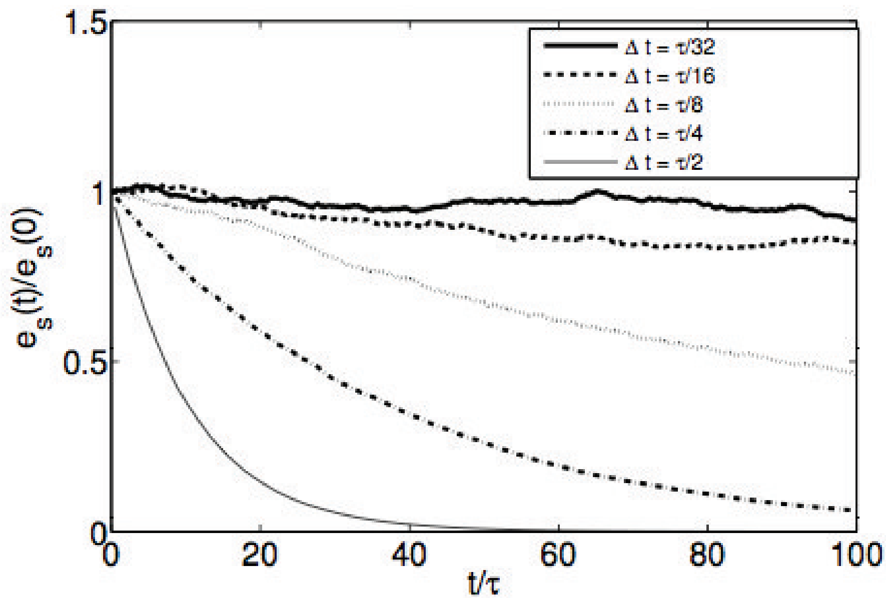
$$\boldsymbol{U}(\boldsymbol{x}^J,t) = \frac{\mathcal{U}^J(t)}{\mathcal{W}^J(t)}$$

$$\boldsymbol{e}_s(\boldsymbol{x}^J,t) = \frac{1}{2}\left(\frac{\mathcal{E}^J(t)}{\mathcal{W}^J(t)} - \boldsymbol{U}^J(t)\cdot\boldsymbol{U}^J(t)\right)$$

Particle Evolution

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

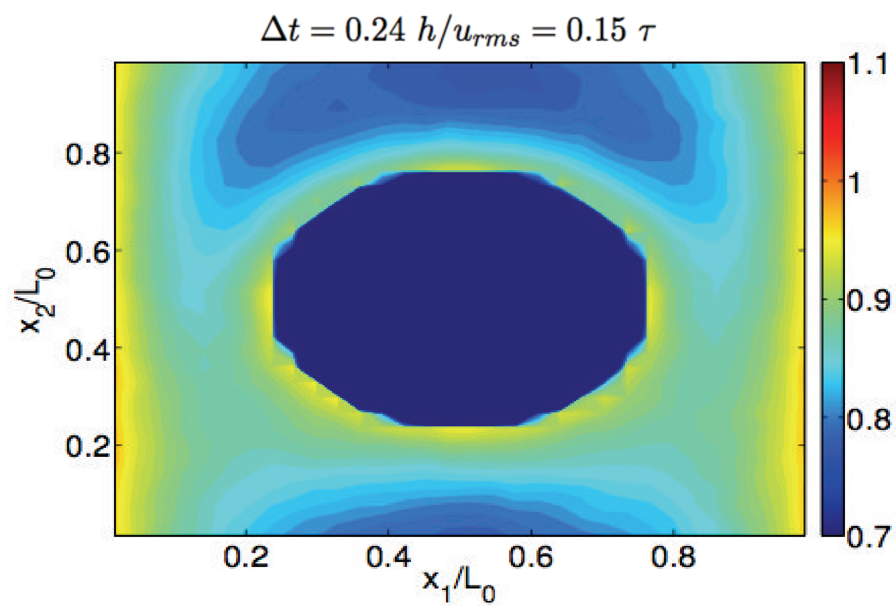
$$\frac{dM_i}{dt} = -\frac{1}{\tau}(M_i - U_i) + \left(\frac{4e_s}{3\tau}\right)^{1/2} \frac{dW_i(t)}{dt} + F_i$$



$$M_i^{n+1} - M_i^n = \left[-\frac{\Delta t}{\tau} M_i^n + \left(\frac{4e_s}{3\tau}\Delta t\right)^{1/2} \xi_i\right]\left[1 - \frac{\Delta t}{2\tau}\right] \quad \text{and}$$

$$\Delta X_i^{n+1} = \frac{\Delta t}{2}\left(M_i^n + M_i^{n+1}\right)$$

Particle Evolution



$$M_i^{n+1} - M_i^n = \left[-\frac{\Delta t}{\tau} M_i^n + \left(\frac{4 e_s}{3\tau} \Delta t \right)^{1/2} \xi_i \right] \left[1 - \frac{\Delta t}{2\tau} \right] \quad \text{and}$$

$$\Delta X_i^{n+1} = \frac{\Delta t}{2} \left(M_i^n + M_i^{n+1} \right)$$

Derivation of New Particle Evolution Scheme

statistically exact (up to 2nd moments) for constant $\boldsymbol{U}$ and e_s for any time step Δt:

without loss of generality, $U_i = F_i = 0$ is assumed

solution of $\frac{dX_i}{dt} = M_i$ and

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

is considered

$$M_i^{n+1} = M_i^n e^{-\Delta t/\tau} + \lim_{N\to\infty} \sum_{k=1}^{N} \xi_{k,i} \left(\frac{4e_s}{3\tau}\frac{\Delta t}{N}\right)^{1/2} e^{-k\Delta t/(N\tau)}$$

$\xi_{k,i}$ are independent, normal distributed random variables

leads to the conditional expectation $\left\langle M_i^{n+1} M_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle = M_i^n M_j^n e^{-2\Delta t/\tau} + \delta_{ij} \lim_{N\to\infty} \sum_{k=1}^{N} \frac{4e_s}{3\tau}\frac{\Delta t}{N} e^{-2k\Delta t/(N\tau)}$

cross products disappear, since $\langle \xi_{k,i}\xi_{h,j} \rangle = \delta_{kh}\delta_{ij}$ and $\langle \xi_{k,i} \rangle = 0$

Derivation of New Particle Evolution Scheme

statistically exact (up to 2nd moments) for constant $\boldsymbol{U}$ and e_s for any time step Δt:

without loss of generality, $U_i = F_i = 0$ is assumed

solution of $\frac{dX_i}{dt} = M_i$ and

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

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$$M_i^{n+1} = M_i^n e^{-\Delta t/\tau} + \lim_{N\to\infty} \sum_{k=1}^{N} \xi_{k,i} \left(\frac{4e_s}{3\tau}\frac{\Delta t}{N}\right)^{1/2} e^{-k\Delta t/(N\tau)}$$

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leads to the conditional expectation $\left\langle M_i^{n+1} M_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle = M_i^n M_j^n e^{-2\Delta t/\tau} + \delta_{ij} \lim_{N\to\infty} \sum_{k=1}^{N} \frac{4e_s}{3\tau}\frac{\Delta t}{N} e^{-2k\Delta t/(N\tau)}$

$$\left\langle M_i^{n+1} M_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle = M_i^n M_j^n e^{-2\Delta t/\tau} + \delta_{ij} \frac{4e_s}{3\tau} \int_0^{\Delta t} e^{-2t/\tau} dt$$
$$= M_i^n M_j^n e^{-2\Delta t/\tau} + \delta_{ij} \frac{2e_s}{3}\left(1 - e^{-2\Delta t/\tau}\right)$$

therefore $M_i^{n+1} = M_i^n e^{-\Delta t/\tau} + \left(\frac{2e_s}{3}\left(1 - e^{-2\Delta t/\tau}\right)\right)^{1/2} \xi_{M,i}$

Derivation of New Particle Evolution Scheme

$$M_i^{n+1} = M_i^n e^{-\Delta t/\tau} + \left(\frac{2e_s}{3} \left(1 - e^{-2\Delta t/\tau}\right) \right)^{1/2} \xi_{M,i}$$

preserves the internal energy $e_s = \dfrac{\langle M_i^n M_i^n \rangle}{2}$ independent of the time step size Δt

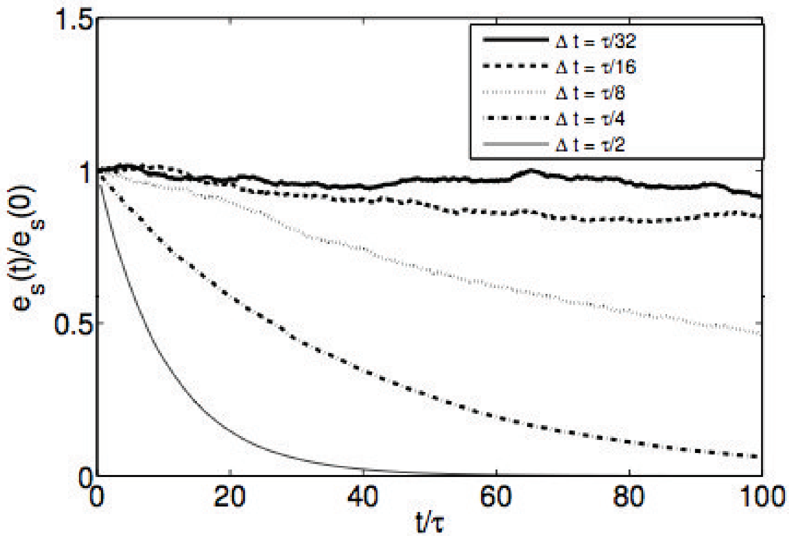
$$\begin{aligned}\langle M_i^{n+1} M_i^{n+1} \rangle &= \langle M_i^n M_i^n \rangle e^{-2\Delta t/\tau} + 2e_s \left(1 - e^{-2\Delta t/\tau}\right) \\ &= \left(\langle M_i^n M_i^n \rangle - 2e_s\right) e^{-2\Delta t/\tau} + 2e_s,\end{aligned}$$

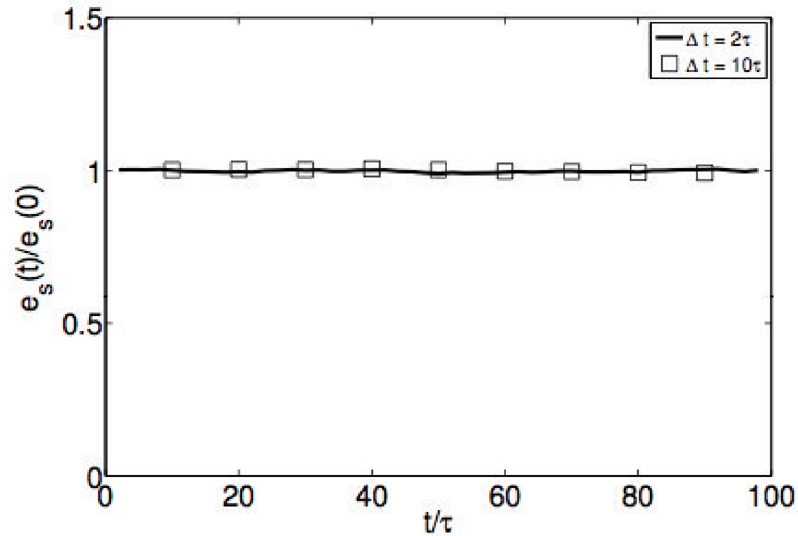
analytically correct correlation coefficient

$$\frac{\langle M_i^{n+1} M_i^n \rangle}{\langle M_i^n M_i^n \rangle} = e^{-\Delta t/\tau}$$

Validation of the Exact Scheme

internal energy:





Derivation of New Particle Evolution Scheme

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

exact particle position scheme

$$\begin{aligned} \Delta X_i^{n+1} &= X_i^{n+1} - X_i^n = M_i^n \tau \left(1 - e^{-\Delta t/\tau}\right) \\ &\quad + \lim_{N\to\infty} \sum_{k=1}^{N} \xi_{k,i} \left(\frac{4e_s}{3\tau}\frac{\Delta t}{N}\right)^{1/2} \tau \left(1 - e^{-k\Delta t/(N\tau)}\right) \end{aligned}$$

$$\begin{aligned} \left\langle \Delta X_i^{n+1} \Delta X_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle &= M_i^n M_j^n \tau^2 \left(1 - e^{-\Delta t/\tau}\right)^2 \\ &\quad + \delta_{ij} \lim_{N\to\infty} \sum_{k=1}^{N} \frac{4e_s}{3\tau}\frac{\Delta t}{N} \tau^2 \left(1 - e^{-k\Delta t/(N\tau)}\right)^2 \end{aligned}$$

Derivation of New Particle Evolution Scheme

$$\left\langle \Delta X_i^{n+1} \Delta X_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle = M_i^n M_j^n \tau^2 \left(1 - e^{-\Delta t/\tau}\right)^2 + \delta_{ij} \lim_{N\to\infty} \sum_{k=1}^{N} \frac{4e_s}{3\tau} \frac{\Delta t}{N} \tau^2 \left(1 - e^{-k\Delta t/(N\tau)}\right)^2$$

which can be written as

$$\begin{aligned}\left\langle \Delta X_i^{n+1} \Delta X_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle &= M_i^n M_j^n \tau^2 \left(1 - e^{-\Delta t/\tau}\right)^2 \\ &\quad + \delta_{ij} \frac{4e_s}{3} \tau \int_0^{\Delta t} \left(1 - 2e^{-t/\tau} + e^{-2t/\tau}\right) dt \\ &= M_i^n M_j^n \tau^2 \left(1 - e^{-\Delta t/\tau}\right)^2 \\ &\quad + \delta_{ij} \frac{2e_s\tau^2}{3} \left(\frac{2\Delta t}{\tau} - \left(1 - e^{-\Delta t/\tau}\right)\left(3 - e^{-\Delta t/\tau}\right)\right)\end{aligned}$$

$$\Delta X_i^{n+1} = M_i^n \tau \left(1 - e^{-\Delta t/\tau}\right)$$

$$+ \left(\frac{2e_s\tau^2}{3} \left(\frac{2\Delta t}{\tau} - \left(1 - e^{-\Delta t/\tau}\right)\left(3 - e^{-\Delta t/\tau}\right)\right)\right)^{1/2} \xi_{X,i}$$

Derivation of New Particle Evolution Scheme

$$M_i^{n+1} = M_i^n e^{-\Delta t/\tau} + \lim_{N\to\infty} \sum_{k=1}^{N} \xi_{k,i} \left(\frac{4e_s}{3\tau} \frac{\Delta t}{N} \right)^{1/2} e^{-k\Delta t/(N\tau)}$$

$$\begin{aligned} \Delta X_i^{n+1} &= X_i^{n+1} - X_i^n = M_i^n \tau \left(1 - e^{-\Delta t/\tau}\right) \\ &\quad + \lim_{N\to\infty} \sum_{k=1}^{N} \xi_{k,i} \left(\frac{4e_s}{3\tau} \frac{\Delta t}{N} \right)^{1/2} \tau \left(1 - e^{-k\Delta t/(N\tau)}\right) \end{aligned}$$

$$\begin{aligned} \left\langle M_i^{n+1} \Delta X_j^{n+1} \middle| \boldsymbol{M}^n \right\rangle &= M_i^n M_j^n \tau \left(e^{-\Delta t/\tau} - e^{-2\Delta t/\tau}\right) \\ &+ \delta_{ij} \lim_{N\to\infty} \sum_{k=1}^{N} \frac{4e_s}{3\tau} \frac{\Delta t}{N} \tau \left(e^{-k\Delta t/(N\tau)} - e^{-2k\Delta t/(N\tau)}\right) \\ &= M_i^n M_j^n \tau \left(e^{-\Delta t/\tau} - e^{-2\Delta t/\tau}\right) \\ &+ \delta_{ij} \frac{4e_s}{3} \int_0^{\Delta t} \left(e^{-t/\tau} - e^{-2t/\tau}\right) dt \\ &= M_i^n M_j^n \tau \left(e^{-\Delta t/\tau} - e^{-2\Delta t/\tau}\right) \\ &+ \delta_{ij} \underbrace{\frac{2e_s\tau}{3} \left(1 - e^{-\Delta t/\tau}\right)^2}_{C} . \end{aligned}$$

Derivation of New Particle Evolution Scheme

$$M_i^{n+1} = M_i^n e^{-\Delta t/\tau} + \overbrace{\Bigg(\underbrace{\frac{2e_s}{3}\left(1 - e^{-2\Delta t/\tau}\right)}_{A}\Bigg)^{1/2} \xi_{M,i}}^{S_{M,i}}$$

$$\Delta X_i^{n+1} = M_i^n \tau \left(1 - e^{-\Delta t/\tau}\right)$$

$$+ \overbrace{\Bigg(\underbrace{\frac{2e_s\tau^2}{3}\left(\frac{2\Delta t}{\tau} - \left(1 - e^{-\Delta t/\tau}\right)\left(3 - e^{-\Delta t/\tau}\right)\right)}_{B}\Bigg)^{1/2} \xi_{X,i}}^{S_{X,i}}$$

$$S'_{M,i} = \left(\frac{C^2}{B}\right)^{1/2} \xi_{1,i} + \left(A - \frac{C^2}{B}\right)^{1/2} \xi_{2,i} \quad \text{and}$$

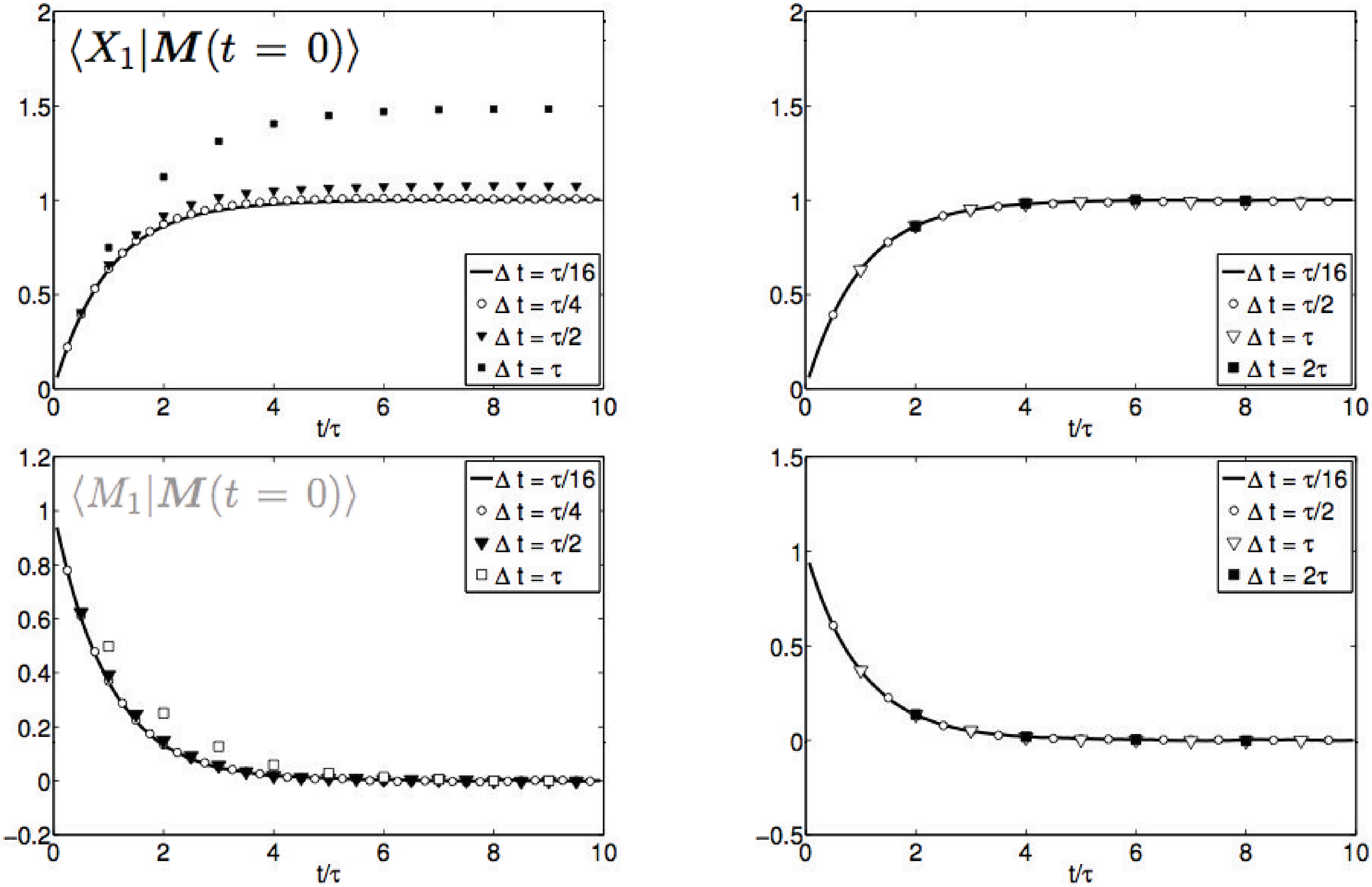
$$S'_{X,i} = (B)^{1/2} \xi_{1,i},$$

$$\langle S'_{M,i} S'_{M,j} \rangle = \langle S_{M,i} S_{M,j} \rangle = \delta_{ij} A \quad \text{and}$$

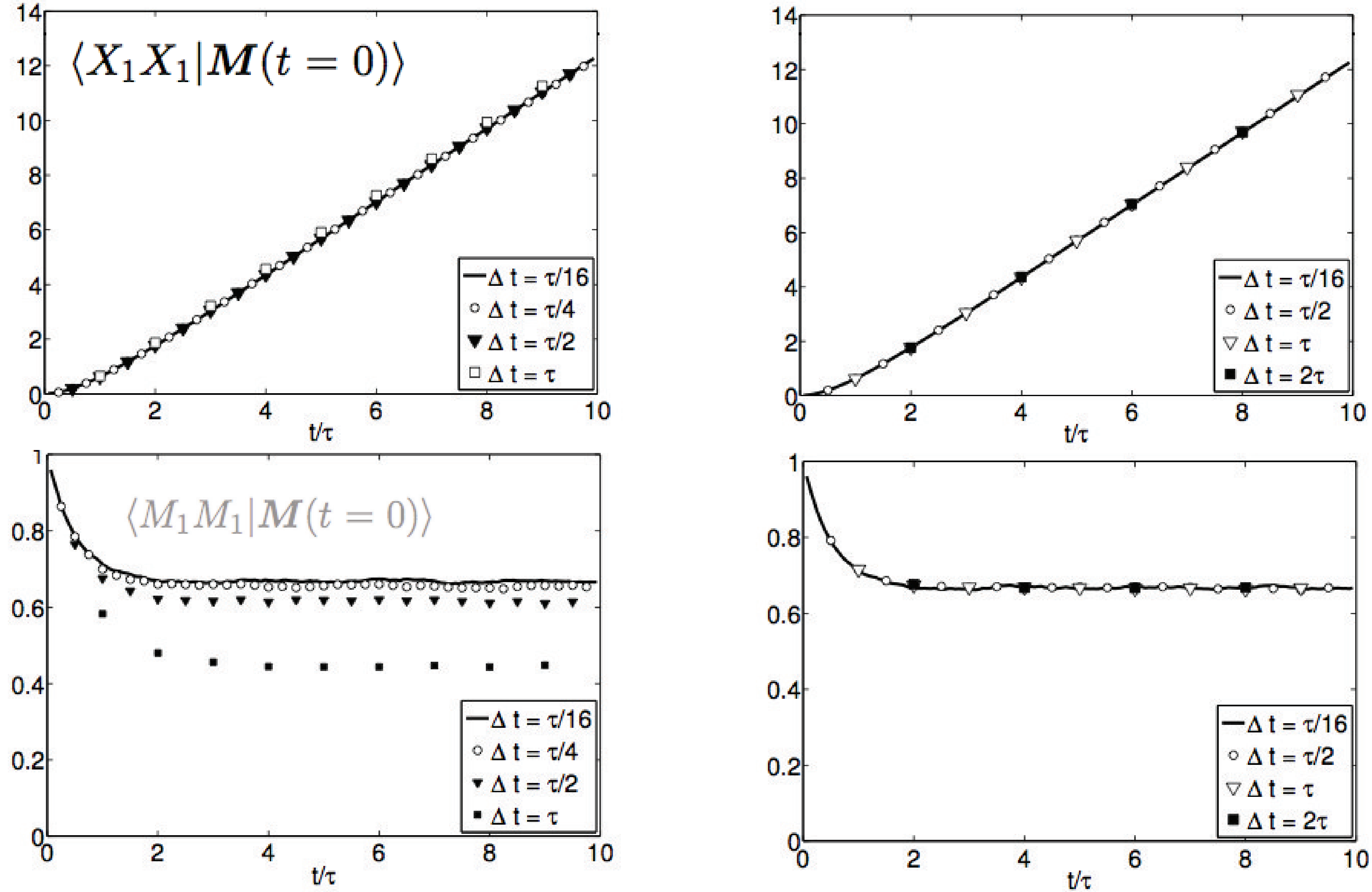
$$\langle S'_{X,i} S'_{X,j} \rangle = \langle S_{X,i} S_{X,j} \rangle = \delta_{ij} B,$$

$$\langle S'_{M,i} S'_{X,j} \rangle = C$$

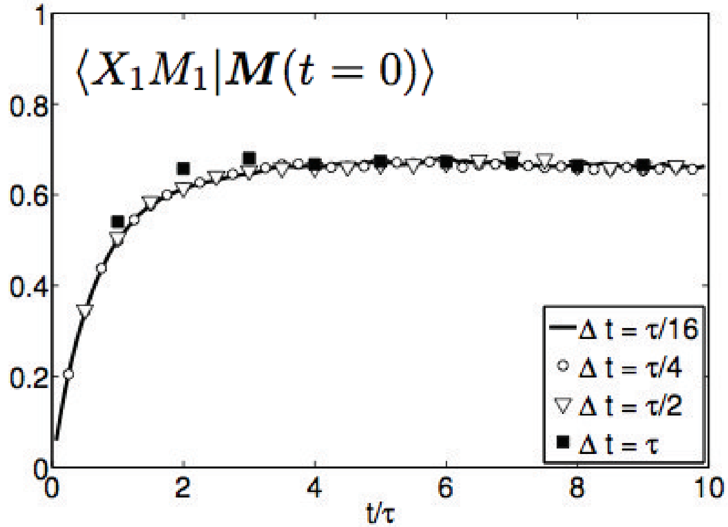
Validation of the Exact Scheme

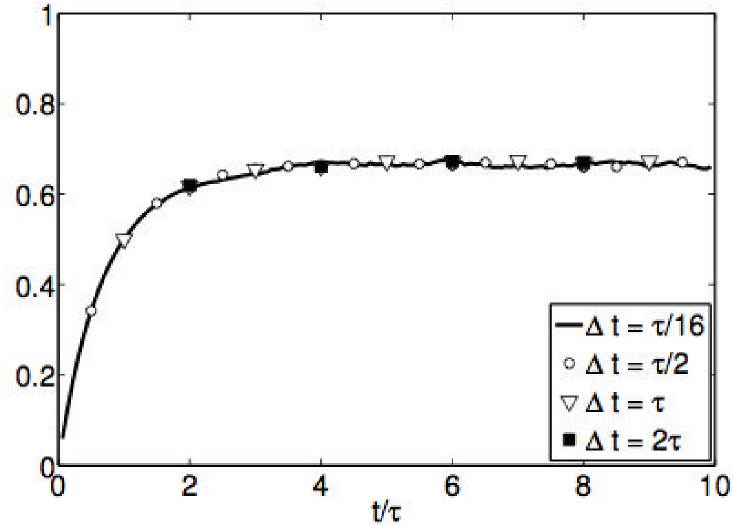


Validation of the Exact Scheme



Validation of the Exact Scheme

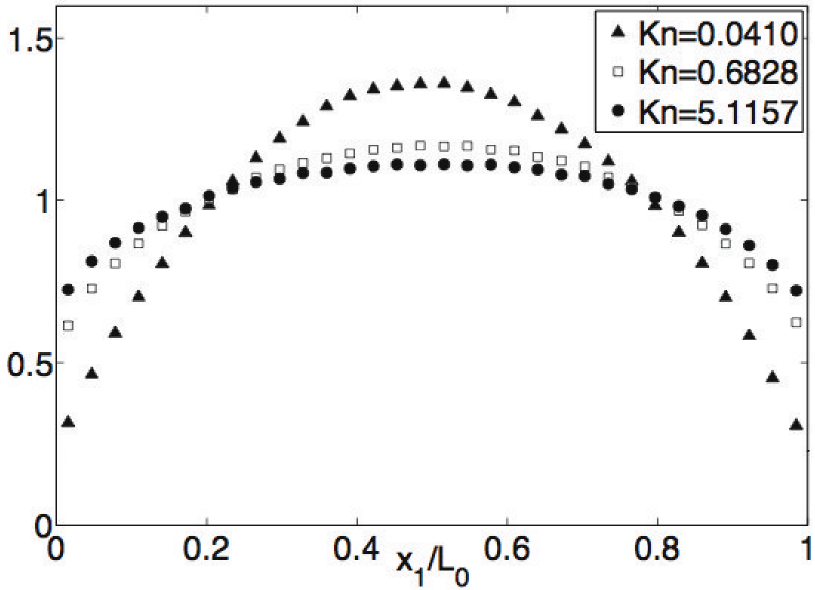


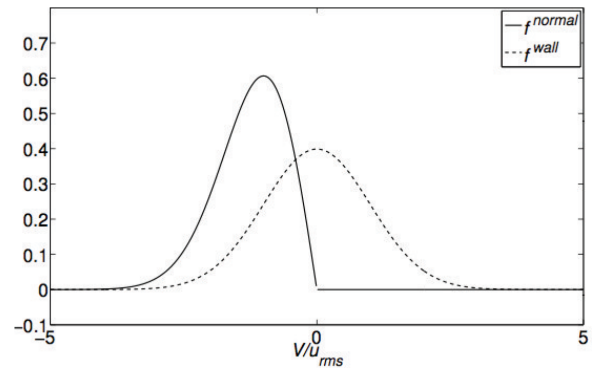


Knudsen Paradox

Periodic-, open- and wall boundary conditions

isothermal wall is treated as an interface between computational and a virtual domain





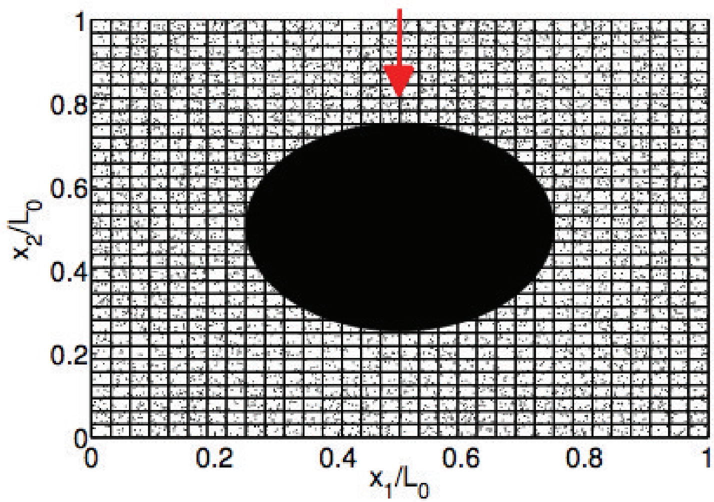
$$f^{wall} = \frac{1}{(2\pi k T^{wall}/m)^{1/2}} \exp\left(-\frac{V_i^2}{2kT^{wall}/m}\right)$$

$$f^{normal} = \frac{-H(-V_n)V_n}{Q} \frac{1}{(2\pi k T^{wall}/m)^{1/2}} \exp\left(-\frac{V_n^2}{2kT^{wall}/m}\right)$$

Flow Around a Cylinder

$$Kn = \lambda/(0.25L_0) = 2\sqrt{RT^{wall}}\tau/L_0 = 0.1$$

$$\hat{F} = FL_0/(RT^{wall}) = 0.4$$

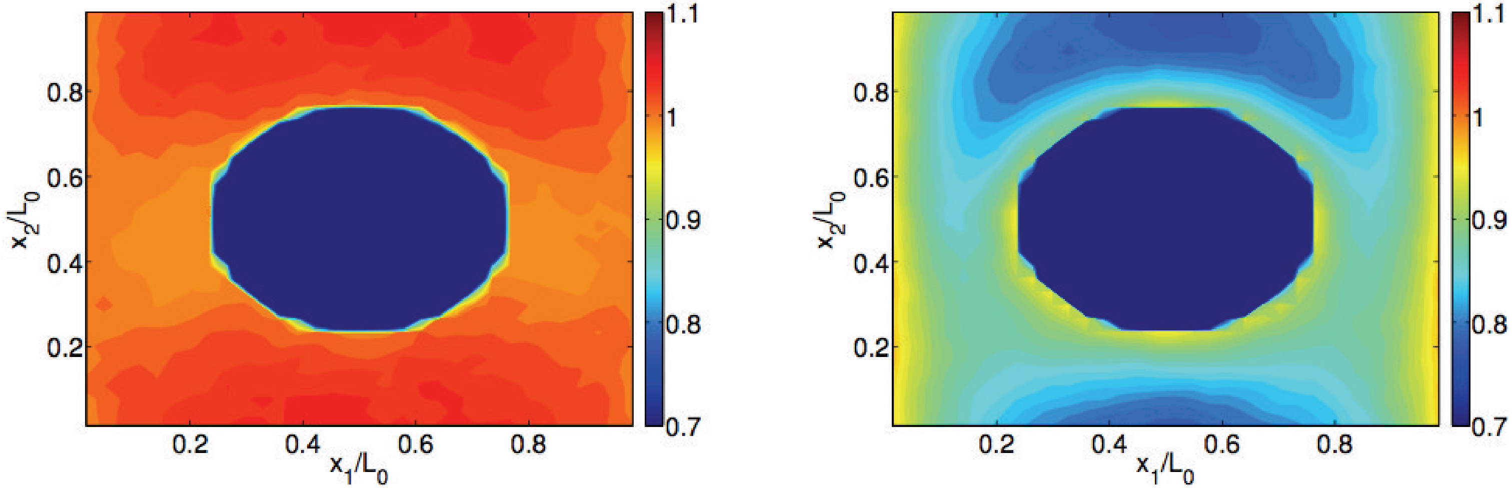


64×64, 32×32, 16×16 and 8×8 grids

10 particles / cell   averaging factor n_a of $10'000$

$$\Delta t = 0.24h/u_{rms}$$

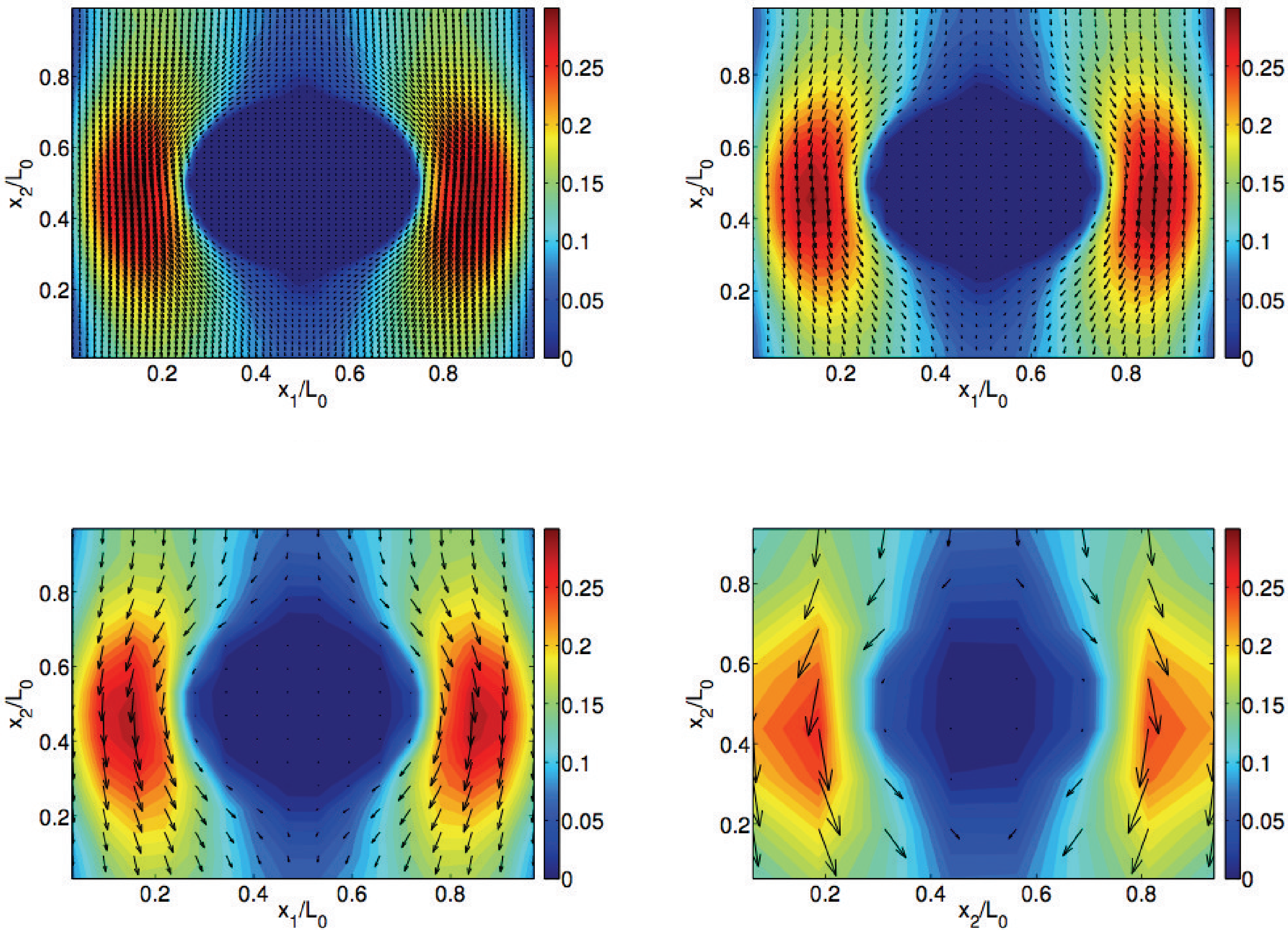
Flow Around a Cylinder



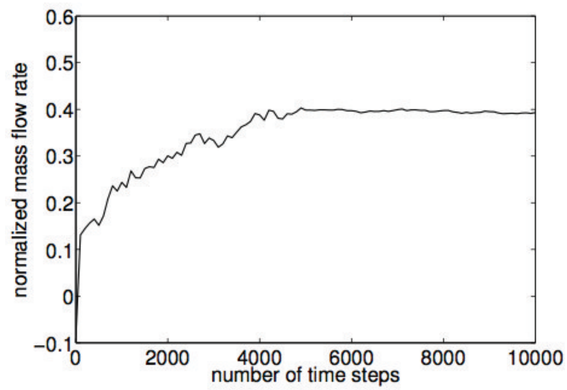
$$32 \times 32 \text{ grid}$$

$$\Delta t = 0.24\ h/u_{rms} = 0.15\ \tau$$

Flow Around a Cylinder



Performance

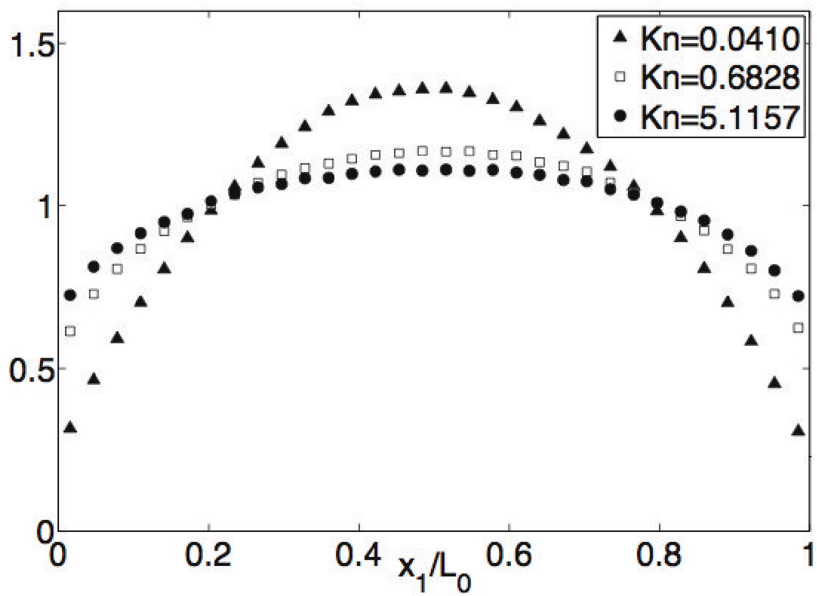


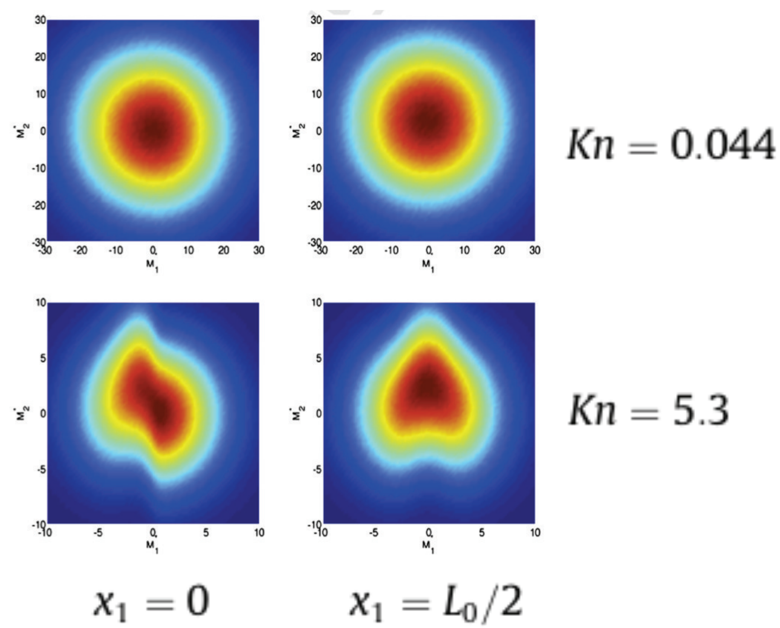
Knudsen paradox (Kn=5.1157): $$\frac{\partial \mathcal{F}}{\partial t} + V_i \frac{\partial \mathcal{F}}{\partial x_i} + \frac{\partial}{\partial V_i} \left\{ \left[F_i - \frac{1}{\tau} (V_i - U_i) \right] \mathcal{F} \right\} = \frac{\partial^2}{\partial V_i \partial V_i} \left\{ \frac{2e_s}{3\tau} \mathcal{F} \right\}$$

number of grid cells	$\hat{J}/\hat{F}$
64	1.315
32	1.317
16	1.327
8	1.341
4	1.383

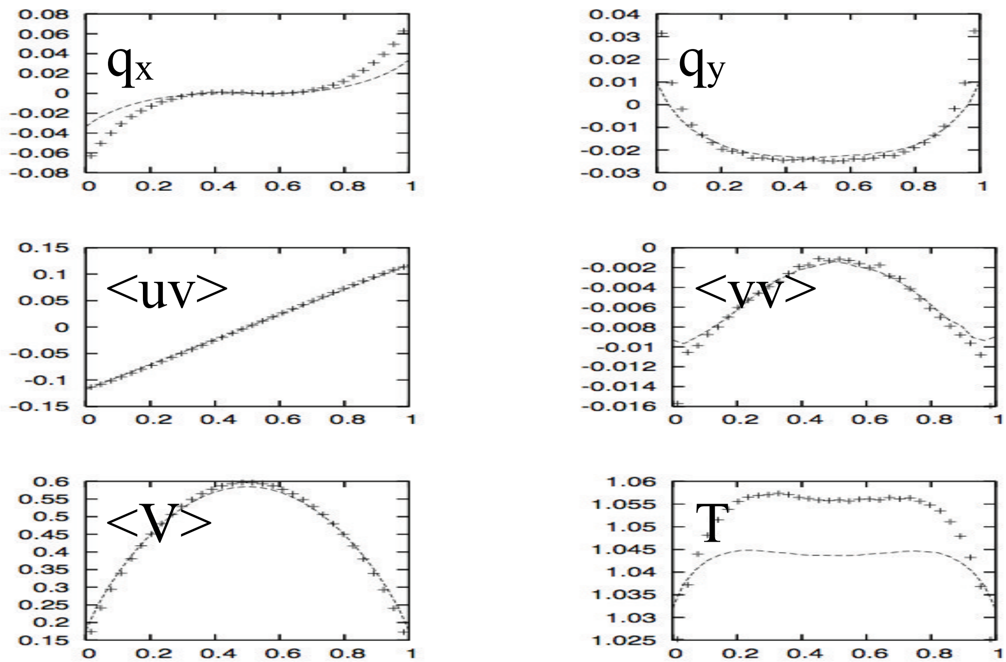
number of grid cells	Δt	$\hat{J}/\hat{F}$
64×64	0.075τ	0.368653
32×32	0.15τ	0.378591
16×16	0.3τ	0.385789
8×8	0.6τ	0.387631

Knudsen Paradox



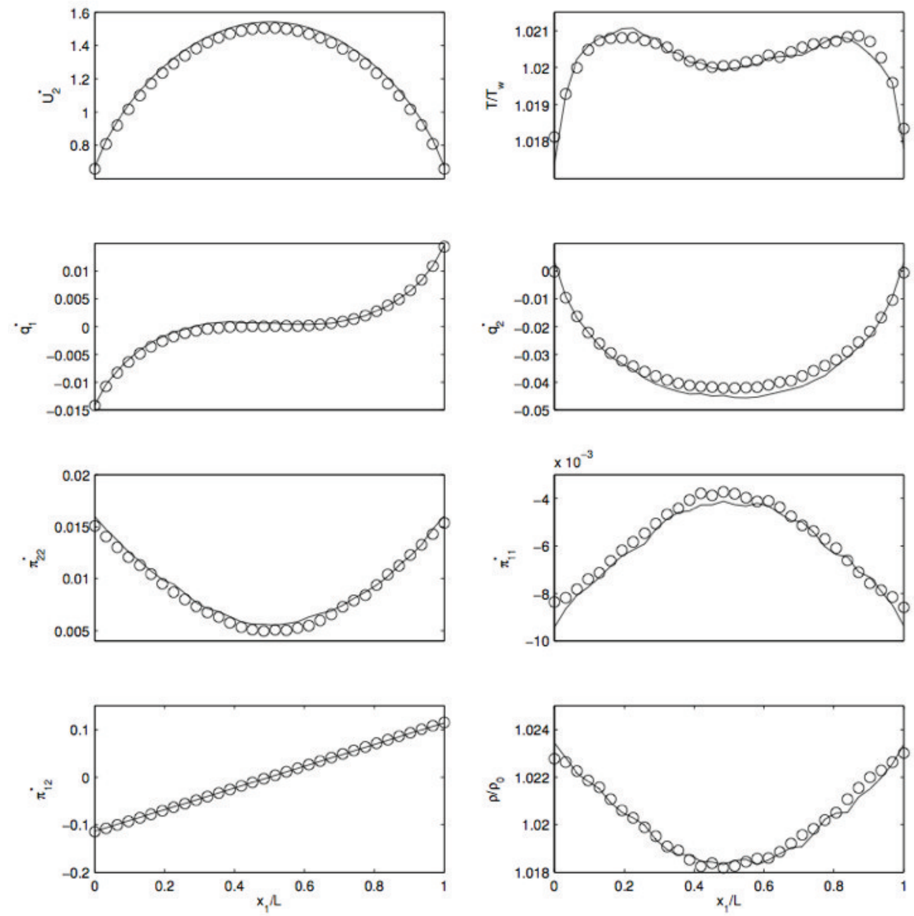


Knudsen Paradox



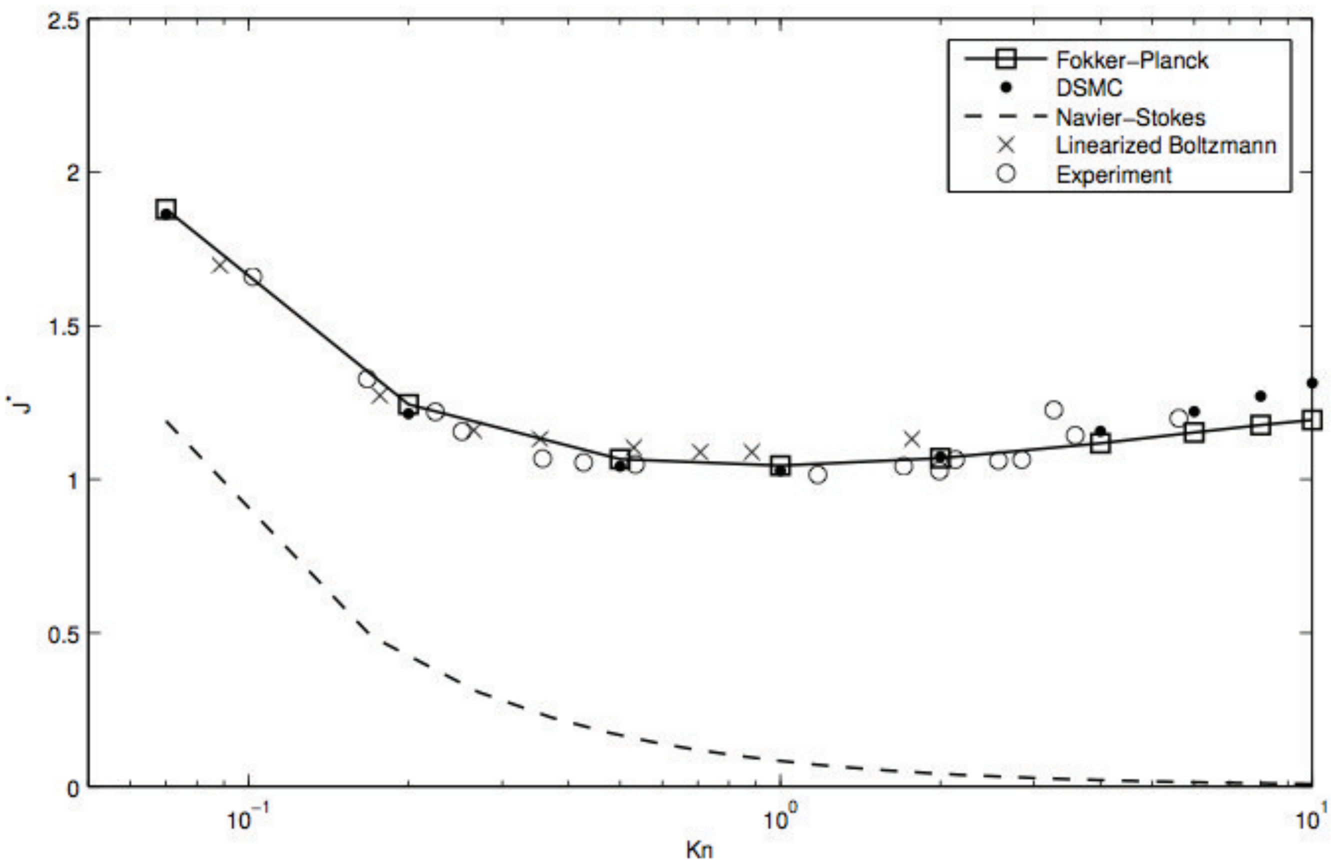
Kn=0.072

Results with a Cubic Model



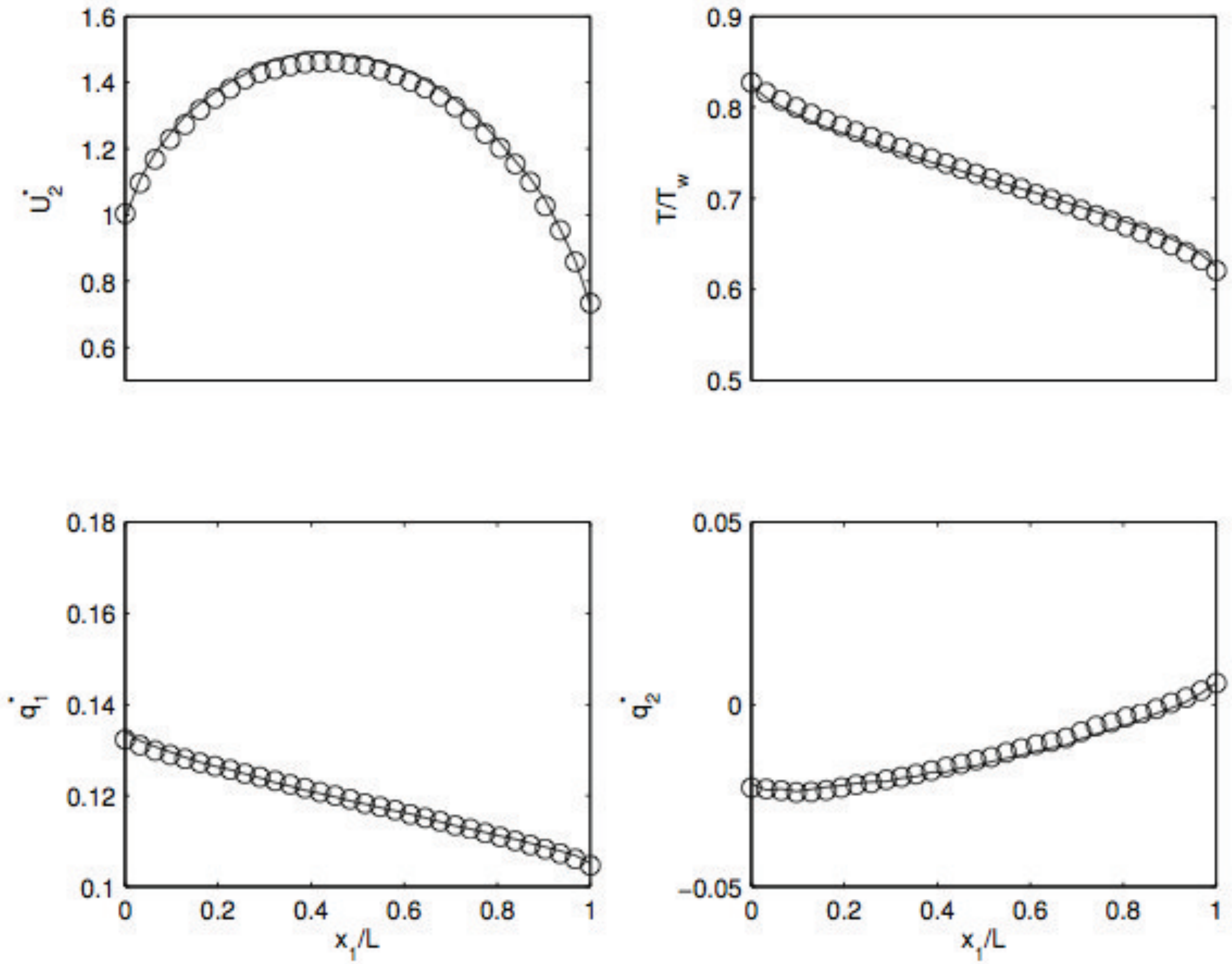
Kn=0.2

Results with a Cubic Model



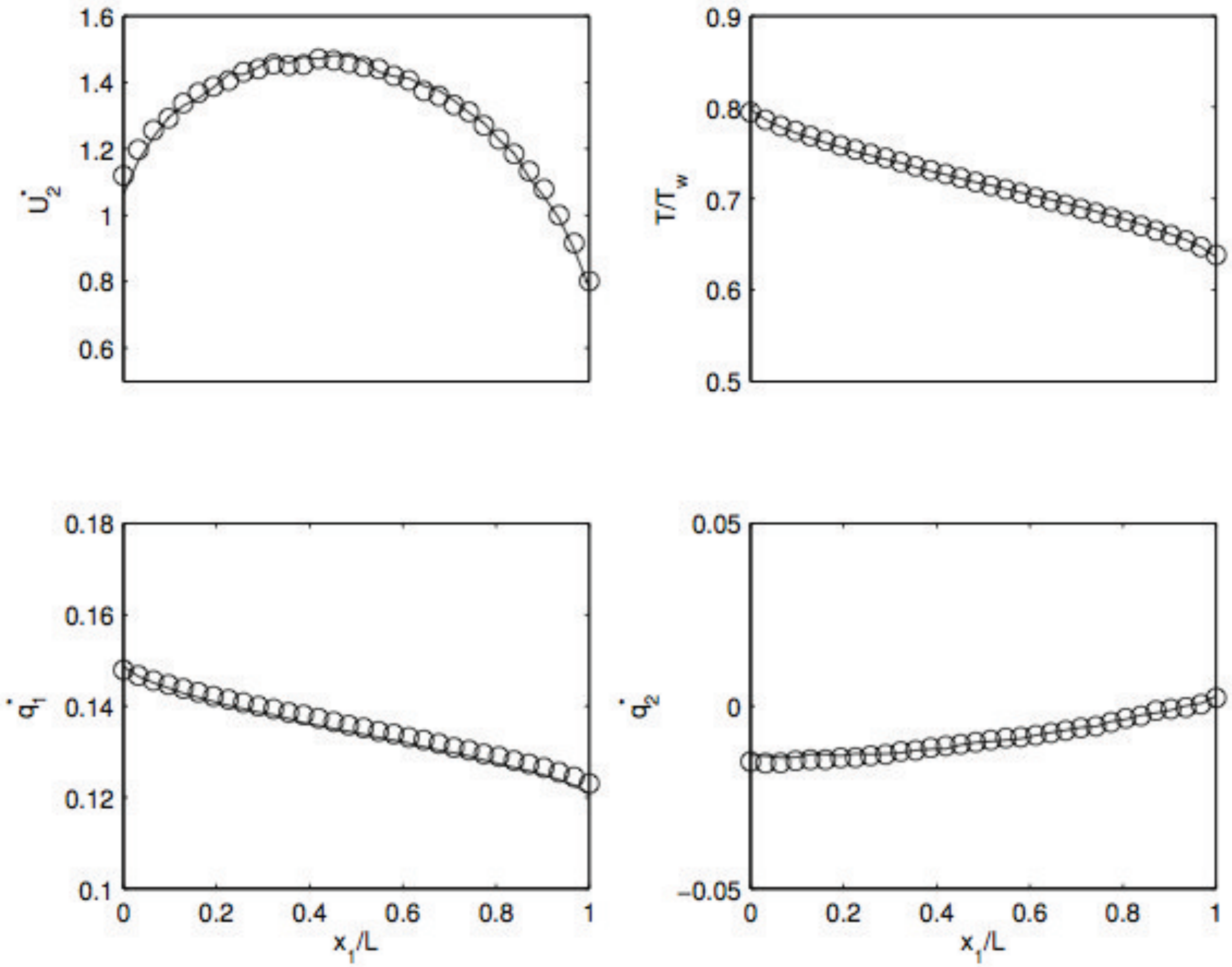
Results with a Cubic Model

Kn=1



Results with a Cubic Model

Kn=2



Multiscale Modeling Framework

Continuum:

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

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

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

Particles:

$$M_i^{n+1} = \dots$$

$$\Delta X_i^{n+1} = \dots$$

Conclusion

- Fokker-Planck collision operator for monatomic gas flow
- Good prediction of Knudsen paradox

- “Exact” particle integration scheme allows for large time steps
- Efficient solution algorithm
- Hybrid framework for multiscale modeling

- Prandtl number problem
- Further validation with Boltzmann and experiments