Unit conversion in LBM

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Outline

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Physical observables and units

physical observables

- usually dimensional, i.e., a number plus a dimension
- measuring means comparing with a reference scale (e.g., measuring tape)

physical units

- fundamental units, e.g., meter, second, kilogram (SI)
- uniquely derived units, e.g., newton, joule, watt

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Computers and physical units

- computers can only process binary numbers
- numbers are dimensionless
- user has to provide unit conversion (physical unit $\leftrightarrow$ number)

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proper unit conversions are required to

1. set up a computer simulation
2. interpret the results afterwards

Hydrodynamics and the law of similarity (1)

dimensionless Navier-Stokes equations

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right)=-\nabla p+\rho\nu\nabla^2\boldsymbol{u}$$

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$$\frac{\partial\tilde{\boldsymbol{u}}}{\partial\tilde{t}}+(\tilde{\boldsymbol{u}}\cdot\tilde{\nabla})\tilde{\boldsymbol{u}}=-\tilde{\nabla}\tilde{p}+\frac{1}{\mathrm{Re}}\tilde{\nabla}^2\tilde{\boldsymbol{u}}$$

$$\tilde{\boldsymbol{u}}=\boldsymbol{u}/u_m,\quad \tilde{p}=p/(\rho u_m^2),\quad \tilde{t}=tu_m/H,\quad \tilde{\nabla}=\nabla H,\quad \mathrm{Re}=\frac{u_m H}{\nu}$$

Hydrodynamics and the law of similarity (1)

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$$\frac{\partial \tilde{\boldsymbol{u}}}{\partial \tilde{t}} + (\tilde{\boldsymbol{u}}\cdot\tilde{\nabla})\tilde{\boldsymbol{u}} = -\tilde{\nabla}\tilde{p} + \frac{1}{\mathrm{Re}}\tilde{\nabla}^2\tilde{\boldsymbol{u}}$$

$$\tilde{\boldsymbol{u}} = \boldsymbol{u}/u_m, \quad \tilde{p} = p/(\rho u_m^2), \quad \tilde{t} = t u_m/H, \quad \tilde{\nabla} = \nabla H, \quad \mathrm{Re} = \frac{u_m H}{\nu}$$

significance of Reynolds number

- only dimensionless number constructible from u_m, H, and ν
- characterizes solutions of Navier-Stokes equations
- flows with same Re are equivalent, even if u_m, H, and ν are different

Hydrodynamics and the law of similarity (2)

- concept of characteristic dimensionless numbers can be generalized to more complicated hydrodynamic problems
- example: presence of diffusive tracer with diffusivity D
- additional dimensionless number (Schmidt number): $\mathrm{Sc} = \nu / D$
- flows with same Re and Sc are equivalent

Hydrodynamics and the law of similarity (2)

- concept of characteristic dimensionless numbers can be generalized to more complicated hydrodynamic problems
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general recommended approach

always find all independent dimensionless numbers for given problem before anything else is done

Conversion principle (1)

for each physical quantity Q, one can write

$$Q = \tilde{Q} \times C_Q$$

Q	$[Q]$	physical value (incl. unit)
$\tilde{Q}$	$[\tilde{Q}] = 1$	dimensionless value
C_Q	$[C_Q] = [Q]$	conversion factor (incl. unit)

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$\tilde{Q}$	$[\tilde{Q}] = 1$	dimensionless value
C_Q	$[C_Q] = [Q]$	conversion factor (incl. unit)

user's task: find all required conversion factors C_Q, but

- relevant dimensionless parameters must be correct
- simulation parameters must be valid

Conversion principle (2)

example for velocity conversion

$$u = \tilde{u} \times C_u$$

$$u = 10\,\frac{\mathrm{m}}{\mathrm{s}}, \quad \tilde{u} = 0.1 \quad \Longrightarrow \quad C_u = 100\,\frac{\mathrm{m}}{\mathrm{s}}$$

Conversion principle (2)

example for velocity conversion

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conversion of dimensionless numbers

dimensionless numbers should generally be invariant, e.g.,

$$\mathrm{Re} = \widetilde{\mathrm{Re}} \quad \Longleftrightarrow \quad C_{\mathrm{Re}} \stackrel{!}{=} 1$$

possible exceptions: e.g., Mach number (next slide).

LBM and the Mach number

- usually, LBM Mach number is larger than in reality
- otherwise, simulations would be too expensive (too many time steps)
- no problem since Ma is not important
- Ma $\stackrel{!}{\ll}$ 1, e.g., Ma < 0.3

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Approaching a hydrodynamic problem

1. identify relevant dimensionless numbers (e.g., Reynolds or Péclet number)
2. write down their definitions, e.g., $\mathrm{Re} = \frac{uH}{\nu}$
3. make use of their invariance during unit conversion, e.g., $\mathrm{Re} = \widetilde{\mathrm{Re}}$ and $C_{\mathrm{Re}} = 1$
4. from this, it is possible to construct a unique set of unit conversions

Approaching a hydrodynamic problem

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4. from this, it is possible to construct a unique set of unit conversions

Explicit examples will be shown later!

Primary conversion factors

for mechanical problems, all quantities have units $m^{q_l} s^{q_t} kg^{q_m}$

quantity	unit	q_l	q_t	q_m
velocity	$\frac{m}{s}$	1	-1	0
force	$kg\frac{m}{s^2}$	1	-2	1
kinematic viscosity	$\frac{m^2}{s}$	2	-1	0

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three independent primary conversion factors required, e.g., for

- length, time, mass
- length, velocity, energy
- length, time, density

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three independent primary conversion factors required, e.g., for

- length, time, mass
- length, velocity, energy
- length, time, density

All other (secondary) conversion factors are uniquely derived.

Finding secondary conversion factors

1. set primary conversion factors,
   e.g., for length, time, and density (C_l, C_t, C_ρ)
2. express secondary units in terms of primary units,
   e.g., for the energy

$$[E] = \frac{\mathrm{kg}\,\mathrm{m}^2}{\mathrm{s}^2} = \frac{\mathrm{kg}}{\mathrm{m}^3}\frac{\mathrm{m}^5}{\mathrm{s}^2} = \frac{[\rho][l]^5}{[t]^2} = \frac{[C_\rho][C_l]^5}{[C_t]^2}$$

3. read off secondary conversion factor, e.g., for the energy

$$C_E = \frac{C_\rho C_l^5}{C_t^2}$$

Finding secondary conversion factors

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$$C_E = \frac{C_\rho C_l^5}{C_t^2}$$

Only the unit of the secondary quantity has to be known!

Outline

1. Introduction & motivation
2. Example discussion
3. Hands-on experience

Gravity-driven planar Poiseuille flow

relevant input parameters

channel height (wall distance)	H
viscosity	ν
density	ρ
gravity (force per volume)	$f = \rho g$

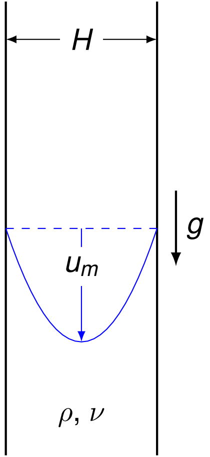
relevant output parameters

maximum velocity (Poiseuille law):

$$u_m = \frac{fH^2}{8\rho\nu}$$

Reynolds number:

$$\mathrm{Re} := \frac{u_m H}{\nu} = \frac{gH^3}{8\nu^2}$$



Physical parameters

example input parameters

channel height	H	$10^{-3}\,\mathrm{m}$
viscosity	ν	$10^{-6}\,\frac{\mathrm{m}^2}{\mathrm{s}}$
density	ρ	$10^{3}\,\frac{\mathrm{kg}}{\mathrm{m}^3}$
gravity	g	$10\,\frac{\mathrm{m}}{\mathrm{s}^2}$

Physical parameters

example input parameters

channel height	H	$10^{-3}\,\mathrm{m}$
viscosity	ν	$10^{-6}\,\frac{\mathrm{m}^2}{\mathrm{s}}$
density	ρ	$10^{3}\,\frac{\mathrm{kg}}{\mathrm{m}^3}$
gravity	g	$10\,\frac{\mathrm{m}}{\mathrm{s}^2}$

resulting output parameters

$$u_m = 1.25\,\frac{\mathrm{m}}{\mathrm{s}}, \quad \mathrm{Re} = 1250$$

These values are defined by the physical problem!

Choose simulation parameters

resolution

$$\tilde{H} = 20, \quad H = 10^{-3}\,\mathrm{m} \quad \Longrightarrow \quad C_H = 5 \times 10^{-5}\,\mathrm{m}$$

Choose simulation parameters

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density

$$\tilde{\rho} = 1, \quad \rho = 10^{3}\,\frac{\mathrm{kg}}{\mathrm{m}^3} \quad \Longrightarrow \quad C_\rho = 10^{3}\,\frac{\mathrm{kg}}{\mathrm{m}^3}$$

Choose simulation parameters

resolution

$$\tilde{H} = 20, \quad H = 10^{-3}\,\mathrm{m} \quad \Longrightarrow \quad C_H = 5 \times 10^{-5}\,\mathrm{m}$$

density

$$\tilde{\rho} = 1, \quad \rho = 10^3\,\frac{\mathrm{kg}}{\mathrm{m}^3} \quad \Longrightarrow \quad C_\rho = 10^3\,\frac{\mathrm{kg}}{\mathrm{m}^3}$$

relaxation time

$$\tau = 0.6$$

The user may choose any other set of parameters!

Make use of Reynolds number

Reynolds number in physical and dimensionless systems

$$\mathrm{Re} = \frac{u_m H}{\nu}, \quad \widetilde{\mathrm{Re}} = \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}}$$

Make use of Reynolds number

Reynolds number in physical and dimensionless systems

$$\mathrm{Re} = \frac{u_m H}{\nu}, \quad \widetilde{\mathrm{Re}} = \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}}$$

equality of Reynolds numbers

$$\mathrm{Re} \stackrel{!}{=} \widetilde{\mathrm{Re}} \quad \Longrightarrow \quad \frac{\nu}{\tilde{\nu}} = \frac{u_m}{\tilde{u}_m} \frac{H}{\tilde{H}} \quad \Longrightarrow \quad C_\nu = C_u C_H$$

Make use of Reynolds number

Reynolds number in physical and dimensionless systems

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consistency check

$$[C_\nu] = [C_u][C_H] = \frac{\mathrm{m}^2}{\mathrm{s}} \quad \checkmark$$

Get time conversion factor

lattice spacing and time step

for convenience, choose $\widetilde{\Delta x} = 1$ and $\widetilde{\Delta t} = 1$

$$\Longrightarrow \quad \Delta x = C_H, \quad \Delta t = C_t$$

Get time conversion factor

lattice spacing and time step

for convenience, choose $\widetilde{\Delta x} = 1$ and $\widetilde{\Delta t} = 1$

$$\implies \quad \Delta x = C_H, \quad \Delta t = C_t$$

LBM viscosity

$$\nu = \left(\tau - \frac{1}{2}\right) c_s^2 \Delta t, \quad c_s^2 = \frac{1}{3}\frac{\Delta x^2}{\Delta t^2} \quad \implies \quad \nu = \underbrace{\frac{\tau - \frac{1}{2}}{3}}_{\tilde{\nu}} \frac{C_H^2}{C_t}$$

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time conversion factor

$$C_t = \frac{\tau - \frac{1}{2}}{3} \frac{C_H^2}{\nu} = 8.\bar{3} \times 10^{-5}\,\mathrm{s}$$

Get velocity conversion factor

secondary conversion factor

$$[u] = \frac{[H]}{[t]} \implies C_u = \frac{C_H}{C_t} \implies C_u = 0.6\,\frac{\mathrm{m}}{\mathrm{s}}$$

Get velocity conversion factor

secondary conversion factor

$$[u] = \frac{[H]}{[t]} \implies C_u = \frac{C_H}{C_t} \implies C_u = 0.6\ \frac{\mathrm{m}}{\mathrm{s}}$$

compute maximum lattice velocity

$$\tilde{u}_m = u_m / C_u \implies \tilde{u}_m = 2.08\bar{3} \quad ϟ$$

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consistency of Reynolds number

$$\mathrm{Re} = \frac{u_m H}{\nu} \stackrel{!}{=} \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}} = 1250 \quad \checkmark$$

Correct simulation parameters

problem

Simulation parameters are consistent,
but not valid for LBM simulations ($\tilde{u}_m \gg 0.3$).

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correction approach

$$C_u = \frac{C_H}{C_t} = \frac{3}{\tau - \frac{1}{2}} \frac{\nu}{C_H}$$

- decrease $C_H \Longrightarrow$ more expensive
- decrease $\tau \Longrightarrow$ LBM may become unstable

User has to find a consistent and valid set of parameters!

Example correction

change resolution and relaxation parameter

- $C_H = 5 \times 10^{-5}\,\mathrm{m} \to C_H^* = 1 \times 10^{-5}\,\mathrm{m}$
- $\tau = 0.6 \to \tau^* = 0.55$

Example correction

change resolution and relaxation parameter

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- $\tau = 0.6 \to \tau^* = 0.55$

corrected velocity conversion factor

$$C_u^* = \frac{3}{\tau^* - \frac{1}{2}} \frac{\nu}{C_H^*} = 6\,\frac{m}{s} \quad \Longrightarrow \quad \tilde{u}_m^* = 0.208\bar{3} \quad \checkmark$$

Example correction

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- $C_H = 5 \times 10^{-5}\,\mathrm{m} \rightarrow C_H^* = 1 \times 10^{-5}\,\mathrm{m}$
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consistency of Reynolds number

$$\mathrm{Re} = \frac{u_m H}{\nu} \overset{!}{=} \frac{\tilde{u}_m^* \tilde{H}^*}{\tilde{\nu}^*} = 1250 \quad \checkmark$$

The user has found a consistent and valid parameter set.

Get force conversion factor

secondary conversion factor

$$[f] = \frac{[\rho][H]}{[t]^2} \implies C_f = \frac{C_\rho C_H}{C_t^2} \implies C_f = 3.6 \times 10^9 \ \frac{\mathrm{N}}{\mathrm{m}^3}$$

Get force conversion factor

secondary conversion factor

$$[f] = \frac{[\rho][H]}{[t]^2} \quad \Longrightarrow \quad C_f = \frac{C_\rho C_H}{C_t^2} \quad \Longrightarrow \quad C_f = 3.6 \times 10^9 \ \frac{\mathrm{N}}{\mathrm{m}^3}$$

compute lattice force density

$$\tilde{f} = f / C_f \quad \Longrightarrow \quad \tilde{f} = 2.\bar{7} \times 10^{-6}$$

Everything for a successful simulation is prepared!

Alternative routes

start with $\tilde{H}$ and $\tilde{u}_m$

1. choose $\tilde{H}$ and $\tilde{u}_m \Longrightarrow C_H, C_u$
2. find viscosity conversion factor $C_\nu = C_H^2/C_t \Longrightarrow \tilde{\nu}$
3. identify relaxation time τ from $\tilde{\nu} = (\tau - \frac{1}{2})/3$
4. find remaining conversion factors & check validity

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start with $\tilde{u}_m$ and τ

1. choose $\tilde{u}_m$ and $\tau \Longrightarrow C_u, \tilde{\nu}$
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3. find length conversion factor $C_H = C_\nu/C_u \Longrightarrow \tilde{H}$
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4. find remaining conversion factors & check validity

and so on...

Outline

Gravity-driven Poiseuille flow with diffusive tracer

relevant input parameters

channel height (wall distance)	H
viscosity	ν
tracer diffusivity	D
density	ρ
gravity (force per volume)	$f = \rho g$

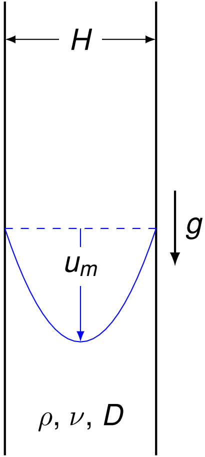
relevant dimensionless parameters

Reynolds number:

$$\mathrm{Re} := \frac{u_m H}{\nu} = \frac{g H^3}{8\nu^2}$$

Schmidt number:

$$\mathrm{Sc} := \frac{\nu}{D}$$



Formulary

dimensionless parameters

$$\mathrm{Re} = \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}} = \frac{\tilde{g}\tilde{H}^3}{8\tilde{\nu}^2}, \quad \mathrm{Sc} = \frac{\tilde{\nu}}{\tilde{D}}$$

dimensionless viscosity and diffusivity

$$\tilde{\nu} = \frac{\tau_\nu - \frac{1}{2}}{3}, \quad \tilde{D} = \frac{\tau_D - \frac{1}{2}}{3}$$

gravity

$$\tilde{f} = \tilde{\rho}\tilde{g}$$

Physical parameters and numerical restrictions

physical parameters

$$\mathrm{Re} = 100, \quad \mathrm{Sc} = 3$$

Physical parameters and numerical restrictions

physical parameters

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numerical restrictions

- relaxation times τ_ν and τ_D shall both be at least 0.55 (stability)
- center velocity shall be $\tilde{u}_m \leq 0.05$ (compressibility)
- system height shall be $\tilde{H} \leq 150$ (efficiency)

Physical parameters and numerical restrictions

physical parameters

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- center velocity shall be $\tilde{u}_m \leq 0.05$ (compressibility)
- system height shall be $\tilde{H} \leq 150$ (efficiency)

task

Find a conclusive and valid set of simulation parameters!

$$\tilde{\rho}, \tau_\nu, \tau_D, \tilde{H}, \tilde{u}_m, \tilde{f}$$

Example solution, part 1

identify minimum relaxation parameters

$$\mathrm{Sc} = \frac{\tilde{\nu}}{\tilde{D}} \quad \Longrightarrow \quad \mathrm{Sc} = \frac{\tau_\nu - \frac{1}{2}}{\tau_D - \frac{1}{2}} \quad \Longrightarrow \quad \tau_\nu = \mathrm{Sc}(\tau_D - 0.5) + 0.5$$

$$\tau_{D,\mathrm{min}} = 0.55, \ \mathrm{Sc} = 3 \quad \Longrightarrow \quad \tau_{\nu,\mathrm{min}} = 0.65$$

Example solution, part 1

identify minimum relaxation parameters

$$\mathrm{Sc} = \frac{\tilde{\nu}}{\tilde{D}} \quad \Longrightarrow \quad \mathrm{Sc} = \frac{\tau_\nu - \frac{1}{2}}{\tau_D - \frac{1}{2}} \quad \Longrightarrow \quad \tau_\nu = \mathrm{Sc}(\tau_D - 0.5) + 0.5$$

$$\tau_{D,\mathrm{min}} = 0.55,\ \mathrm{Sc} = 3 \quad \Longrightarrow \quad \tau_{\nu,\mathrm{min}} = 0.65$$

identify minimum resolution

$$\mathrm{Re} = \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}} \quad \Longrightarrow \quad \tilde{H} = \mathrm{Re}\frac{\tau_\nu - 0.5}{3\tilde{u}_m}$$

$$\tau_{\nu,\mathrm{min}} = 0.65,\ \tilde{u}_{m,\mathrm{max}} = 0.05,\ \mathrm{Re} = 100 \quad \Longrightarrow \quad \tilde{H}_{\mathrm{min}} = 100$$

Example solution, part 2

chosen set of simulation parameters

$$\tau_\nu = 0.65, \quad \tau_D = 0.55, \quad \tilde{H} = 100, \quad \tilde{u}_m = 0.05$$

Example solution, part 2

chosen set of simulation parameters

$$\tau_\nu = 0.65, \quad \tau_D = 0.55, \quad \tilde{H} = 100, \quad \tilde{u}_m = 0.05$$

validity and consistency already assured

$$\mathrm{Re} = \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}} = 100, \quad \mathrm{Sc} = \frac{\tilde{\nu}}{\tilde{D}} = 3 \quad \checkmark$$

Example solution, part 2

chosen set of simulation parameters

$$\tau_\nu = 0.65, \quad \tau_D = 0.55, \quad \tilde{H} = 100, \quad \tilde{u}_m = 0.05$$

validity and consistency already assured

$$\text{Re} = \frac{\tilde{u}_m \tilde{H}}{\tilde{\nu}} = 100, \quad \text{Sc} = \frac{\tilde{\nu}}{\tilde{D}} = 3 \quad \checkmark$$

set density

$$\tilde{\rho} = 1 \quad \text{(arbitrary)}$$

Example solution, part 2

chosen set of simulation parameters

$$\tau_\nu = 0.65, \quad \tau_D = 0.55, \quad \tilde{H} = 100, \quad \tilde{u}_m = 0.05$$

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set density

$$\tilde{\rho} = 1 \qquad \text{(arbitrary)}$$

set gravity

$$\mathrm{Re} = \frac{\tilde{g}\tilde{H}^3}{8\tilde{\nu}^2} \quad \Longrightarrow \quad \tilde{f} = \tilde{\rho}\tilde{g} = \frac{8\tilde{\rho}\tilde{\nu}^2}{\tilde{H}^3}\mathrm{Re} = 2 \times 10^{-6}$$

Further comments

- systems with identical Re and Sc are equivalent
  $\Longrightarrow$ no explicit conversion factors required at this point!
- scale can be introduced afterwards, e.g.,

$$H = 10^{-3}\,\mathrm{m} \quad \Longrightarrow \quad C_H = 10^{-5}\,\mathrm{m}$$

- all other conversion factors are then obtained as in the example discussion