Why Should We Be Interested in Hydrodynamics?

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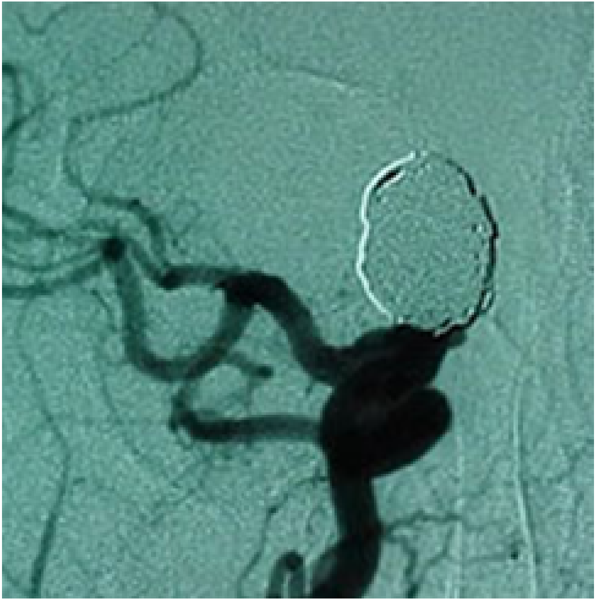
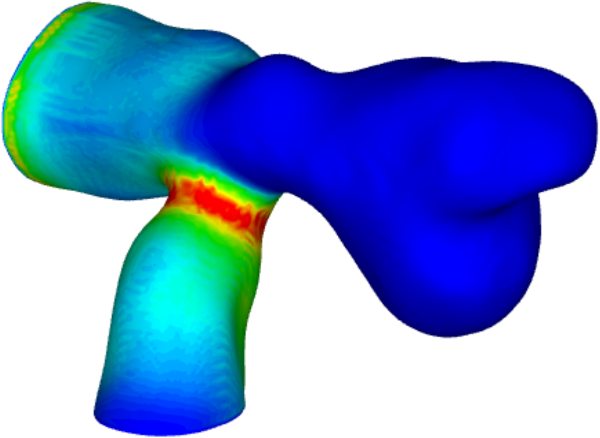
Outline

- Prelude: Some examples;
- Some Mathematics
- Modeling Flows
- Our Research Activities
- Conclusions

Medical Applications



Medical Applications



How Owl Catch Mouse?

Owl → Quiet UAV

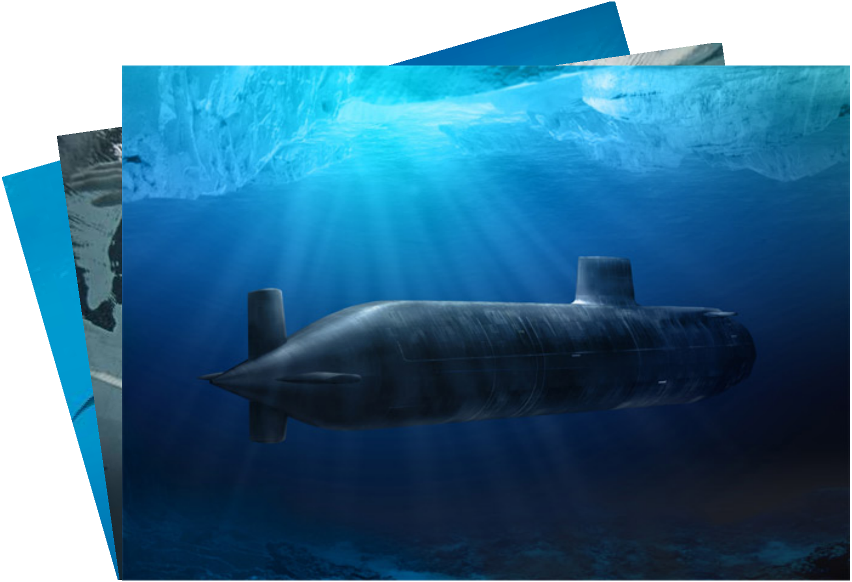
Owl → Quiet UAV, Car

Owl → Quiet UAV, Car, and Airplane

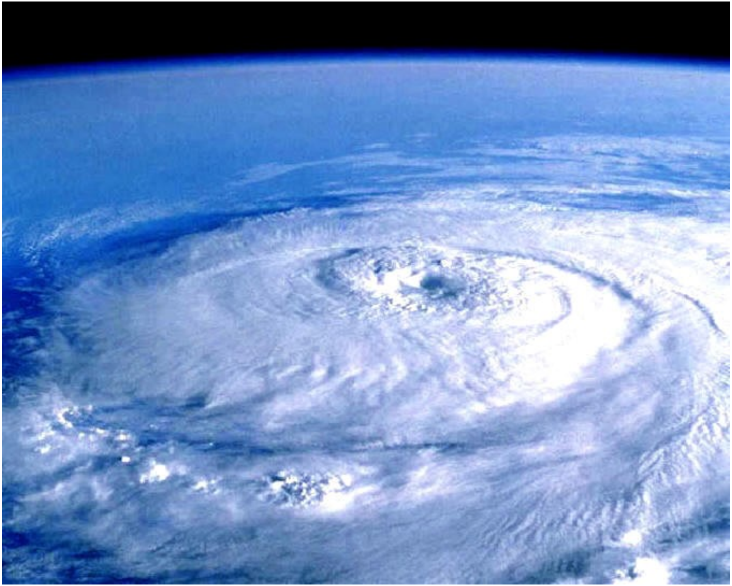
How Dolphin Swim and Swim Fast?

Dolphin → Speedo Swimsuit

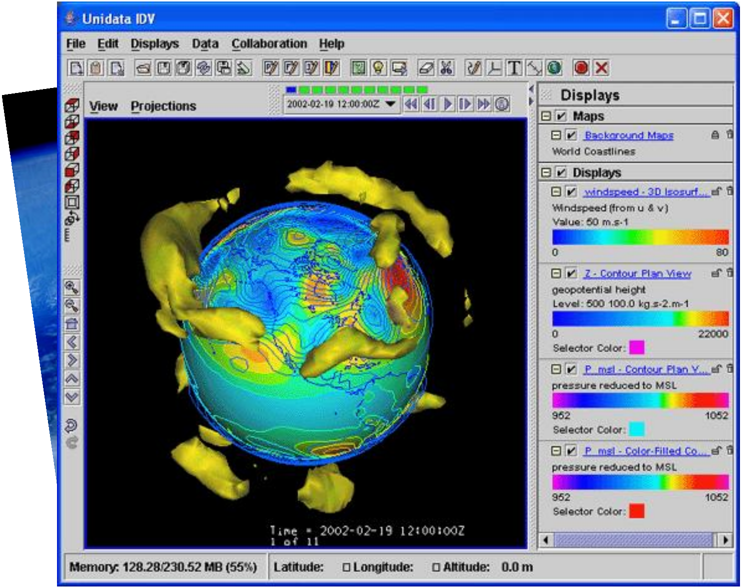
Dolphin → Speedo Swimsuit and Submarine



Weather Prediction

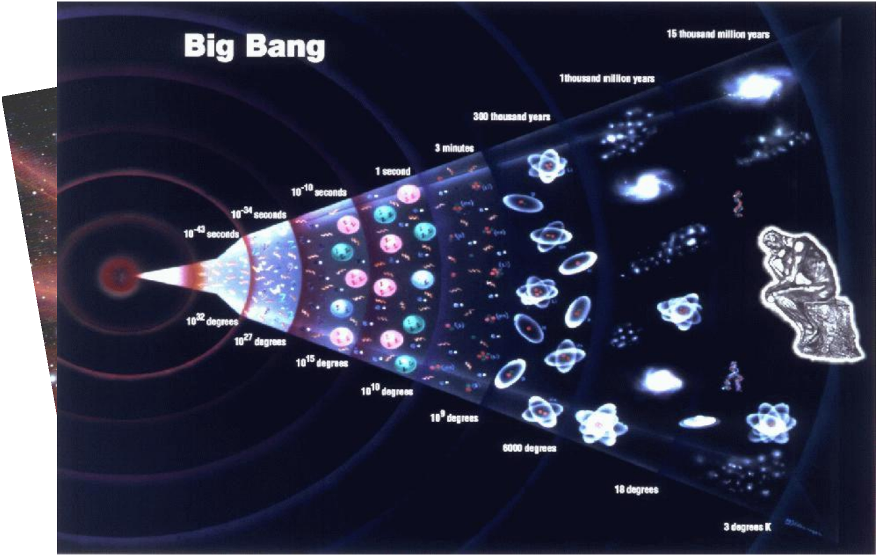


Weather Prediction



Big Bang, Cosmology

Big Bang, Cosmology



Navier-Stokes Equations: Continuum Theory

Conservation laws of mass, momentum, and energy:

$$\partial_t \rho + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u} = 0 \tag{1a}$$

$$\rho \partial \boldsymbol{u} + \rho \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\boldsymbol{\nabla} \cdot \mathsf{P} \tag{1b}$$

$$\rho \partial_t e + \rho \boldsymbol{u} \cdot \boldsymbol{\nabla} e = -\mathsf{P} : \boldsymbol{\nabla} \boldsymbol{u} - \boldsymbol{\nabla} \cdot \boldsymbol{q} \tag{1c}$$

$$\mathsf{P}_{\alpha\beta} := p \delta_{\alpha\beta} - \mu \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{3} \delta_{\alpha\beta} \boldsymbol{\nabla} \cdot \boldsymbol{u} \right) - \zeta \delta_{\alpha\beta} \boldsymbol{\nabla} \cdot \boldsymbol{u}$$

$$\boldsymbol{q} = -\kappa \boldsymbol{\nabla} T, \quad e = e(T), \quad p = p(\rho, T)$$

Dimensionless Navier-Stokes equations (similarity law):

$$\rho \partial \boldsymbol{u} + \rho \boldsymbol{u} \cdot \boldsymbol{\nabla} \boldsymbol{u} = -\frac{1}{\gamma \mathrm{Ma}^2} \boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}} \boldsymbol{\nabla} \cdot \mathsf{S} \tag{2a}$$

$$\rho \partial_t e + \rho \boldsymbol{u} \cdot \boldsymbol{\nabla} e = -\frac{1}{\gamma \mathrm{Ma}^2} p \boldsymbol{\nabla} \cdot \boldsymbol{u} + \frac{1}{\alpha} \nabla^2 T + \frac{1}{\mathrm{Re}} \mathsf{S} : \boldsymbol{\nabla} \boldsymbol{u} \tag{2b}$$

$$\alpha = (\gamma - 1) \mathrm{Pr} \mathrm{Ma} \mathrm{Re}$$

Hierarchy of Scales and PDEs

Microscopic Scale

$$\dot{q}_k = \frac{\partial H}{\partial p_k},\ \dot{p}_k = -\frac{\partial H}{\partial q_k}$$

$$H = \sum_{k=1}^{(D+K)N} p_k^2 + V$$

$$i\hbar\dot{\psi} = \mathcal{H}\psi$$

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\boldsymbol{\nabla}_j^2 + V$$

$$h \approx 6.62 \cdot 10^{-34}(\mathrm{J} \cdot \mathrm{s})$$

$$c \approx 2.99 \cdot 10^{8}(\mathrm{m/s})$$

$$a \approx 5 \cdot 10^{-11}(\mathrm{m})$$

$$t_a \approx 2.41 \cdot 10^{-17}(\mathrm{s})$$

$$m \approx 10^{-27}(\mathrm{kg})$$

$$N = 1,\, 2,\, \ldots,\, N_0$$

Mesoscopic Scale

$$\partial_t f + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} f = \frac{1}{\varepsilon}Q(f, f)$$

$$f = f(\boldsymbol{x},\, \boldsymbol{\xi},\, t)$$

$$\varepsilon = \mathrm{Kn} = \frac{\ell}{L},\ \mathrm{Ma} = \frac{U}{c_s}$$

$$k_B \approx 1.38 \cdot 10^{-23}(\mathrm{J/^\circ K})$$

$$\ell \approx 10^2 - 10^3\ (\text{Å})$$

$$\approx 10 - 100\ (\mathrm{nm})$$

$$\tau \approx 10^{-10}(\mathrm{s})$$

$$c_s \approx 300\ (\mathrm{m/s})$$

$$N \gg 1$$

Macroscopic Scale

$$\rho D_t \boldsymbol{u} = -\boldsymbol{\nabla} p + \frac{1}{\mathrm{Re}}\boldsymbol{\nabla}\cdot\sigma$$

$$D_t = \partial_t + \boldsymbol{u}\cdot\boldsymbol{\nabla}$$

$$\sigma = \frac{\rho\nu}{2}[(\boldsymbol{\nabla}\boldsymbol{u}) + (\boldsymbol{\nabla}\boldsymbol{u})^\dagger] + \frac{2\rho\zeta}{D}\mathsf{I}(\boldsymbol{\nabla}\cdot\boldsymbol{u})$$

$$\mathrm{Re}_\delta = \frac{UL}{\nu} \sim \frac{\mathrm{Ma}}{\mathrm{Kn}}$$

$$\nu \approx 10^{-6} - 10^{-4}\ (\mathrm{m^2/s})$$

$$\mathrm{Kn} \approx 0 \qquad \mathrm{Ma} < 10^3$$

$$L \geq 10^{-5}(\mathrm{m}) = 10(\mu\mathrm{m})$$

$$T \geq 10^{-4}(\mathrm{s})$$

$$N \geq N_A \approx 6.02 \cdot 10^{23}$$

In the Course of Hydrodynamic Events ...

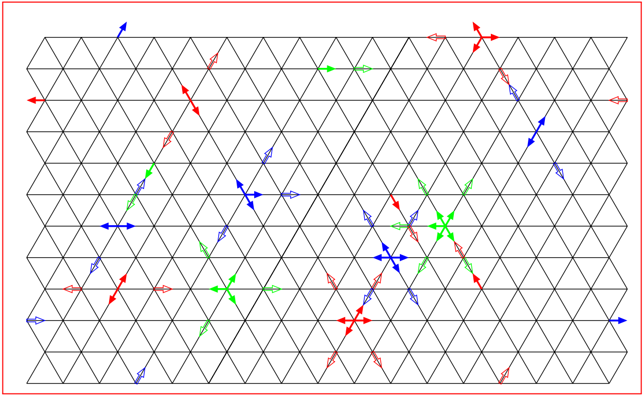
Ma (Mach) and Kn (Knudsen) characterize nonequilibrium

Van Karmen relation based on Navier-Stokes equation ($\mathrm{Kn}=O(\varepsilon)$): $\mathrm{Ma}=\mathrm{Re}\cdot\mathrm{Kn}$			
	$\mathrm{Re}\ll 1$	$\mathrm{Re}\approx 1$	$\mathrm{Re}\gg 1$
$\mathrm{Ma}\ll 1$	Stokes Flows $\mathrm{Ma}=O(\varepsilon^2)$, $\mathrm{Re}=O(\varepsilon)$	Incompressible Navier-Stokes Flows $\mathrm{Ma}=O(\varepsilon)$, $\mathrm{Re}=O(1)$	Incompressible Navier-Stokes Flows $\mathrm{Ma}=O(\varepsilon^{1-\alpha})$, $\mathrm{Re}=O(\varepsilon^{-\alpha})$
$\mathrm{Ma}\approx 1$			Sub/Transonic Flows $\mathrm{Ma}=O(1)$, $\mathrm{Re}=O(\varepsilon^{-1})$
$\mathrm{Ma}\gg 1$			Super/Hypersonic Flows $\mathrm{Ma}=O(\varepsilon^{-1})$, $\mathrm{Re}=O(\varepsilon^{-2})$

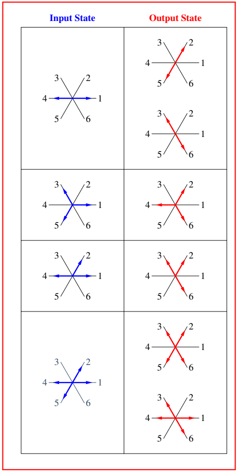
With the framework of kinetic theory (Boltzmann equation)			
Hydrodynamics	Slip Flow	Transitional	Free Molecular
$\mathrm{Kn}<10^{-3}$	$10^{-3}<\mathrm{Kn}<10^{-1}$	$10^{-1}<\mathrm{Kn}<10$	$10<\mathrm{Kn}$

An intuitive system of fictitious particles on a Lattice

Evolution from t (solid arrows) to $t+1$ (hollow arrows):

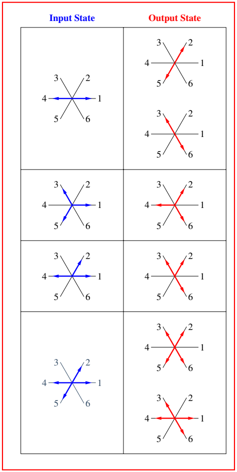


FHP-LGA Collision Rules



$$N_\alpha(\boldsymbol{x}_i + \boldsymbol{e}_\alpha,\, t+1) = N_\alpha(\boldsymbol{x}_i,\, t) + C_\alpha(\{N_\beta\})$$

FHP-LGA Collision Rules



Binary Representation of FHP LGA Collision Rules

Input State	Output State
001001	010010 100100
010101	101010
001011	100110
011011	110110 101101

Why should LGCA work?

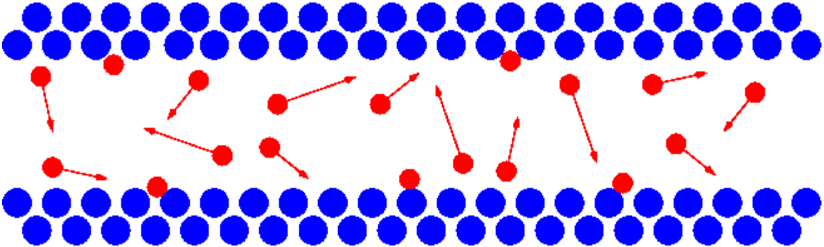
"*We have noticed in nature that the behavior of a fluid depends very little on the nature of the individual particles in that fluid. For example, the flow of sand is very similar to the flow of water or the flow of a pile of ball bearings. We have therefore taken advantage of this fact to invent a type of imaginary particle that is especially simple for us to simulate. This particle is a perfect ball bearing that can move at a single speed in one of six directions. The flow of these particles on a large enough scale is very similar to the flow of natural fluids.*"

— Richard P. Feynman (1918 – 1988)

ODU Research: Complex Bio-Fluids, Lab-on-a-Chip

- Prof. S. Qian *et al.* (Dept. of Mech. & Aerospace Eng.): Experiments (MEMS) to separate particles by size or charge;
- Prof. Y. Peng *et al.* (Dept. of Math. & Stat.): Simulations of a particle moving in sediment or in a channel.

ODU Research: Gas Flow in MEMS

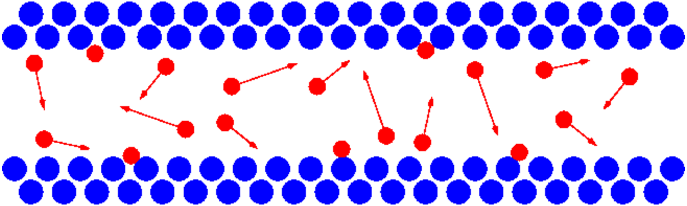


Gas Flow in MEMS: What's the problem?

The scales in this problem:

- Device size: $10^{-6}\text{m} = 1\mu\text{m}$
  The mean-free-path of air: $70 \cdot 10^{-9}\text{m} = 70\text{nm}$
  The *effective* air molecular diameter: $\sigma \approx 3 \cdot 10^{-10}\text{m} = 0.1\text{nm}$
  Typical hydrodynamic time scale: $10^{-3}\text{s} - 10^{-9}\text{s}$
- To consider molecule-surface interaction, one must use Molecular Dynamics (MD) simulations. Typical time step size for MD:

$$\tau \sim \sigma\sqrt{m/\epsilon} \sim 10^{-12}\text{s} = 1\text{ps}$$

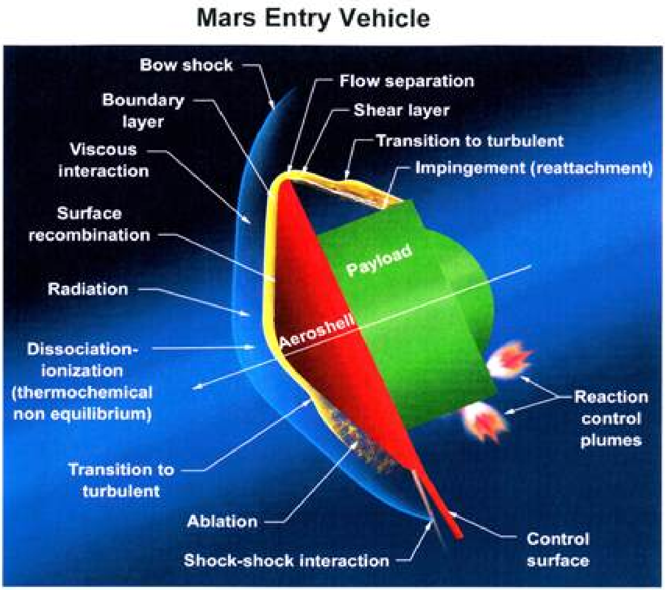


Gas Flow in MEMS: A Possible Solution

- Not to directly couple MD and CFD!
- Use MD to compute the *mean-field* potential near the wall;
- Use kinetic schemes to include the *mean-field* potential obtained from the MD;

The goal is to drastically reduce computational time.

ODU Research: Hypersonic Rarefied Gas Flow



Hypersonic Rarefied Gas Flow

The hypersonic rarefied gas flows are strongly nonequilibrium:

- Large Ma: strong and complex shock-shock and shock-boundary layer interactions;
- Large Kn: Navier-Stokes equations no longer valid;

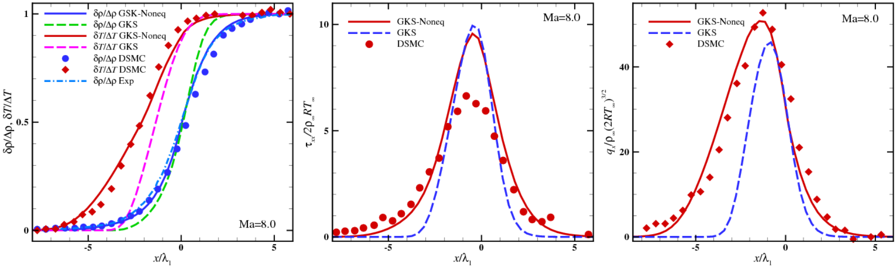
Established method for nonequilibrium flows:

- Direct Monte Carlo simulations (DSMC), a stochastic method;
- Deterministic solution methods of the Boltzmann equation.

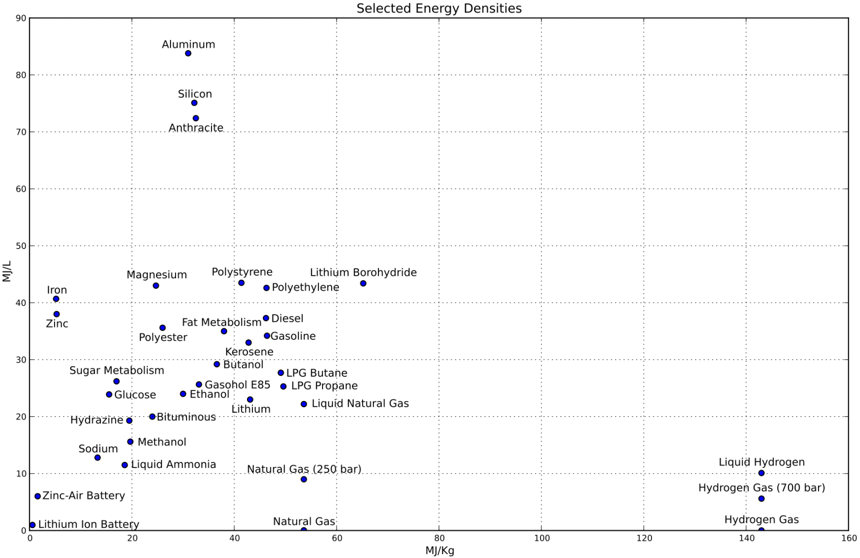
Our strategy: kinetic methods — Extending the Navier-Stokes equations based on the Boltzmann equation.

Hypersonic Rarefied Gas Flow: Shock at Ma = 8.0

The *gas-kinetic scheme* based on the Boltzmann equation can accurately and efficiently predict shock thickness (about a few mean-free paths), the stress and heat flux across a shock.



A New Direction: Energy Storage



A New Direction: Energy Storage

Nanoporous energy absorption system (NEAS), *e.g.*, silica nanoporous material:

- Porosity $30\% \sim 90\%$, high specific pore area $> 1,000$ (m^2/g)
- Extremely high specific energy absorption: > 140.0 (J/g), compared to Li-Battery $\approx 2,500$ (J/g), TNT $\approx 4,610$ (J/g), gasoline $\approx 46,400$ (J/g).

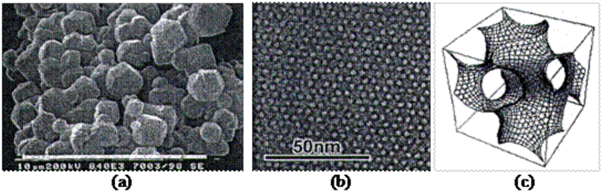
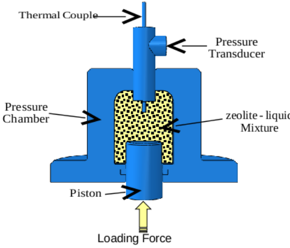


Fig.4 (a) SEM microscopy of the mesoporous silica particles; (b) TEM microscopy of the particle surface; (c) the mesoporous structure (Terasaki, et al., 2002).



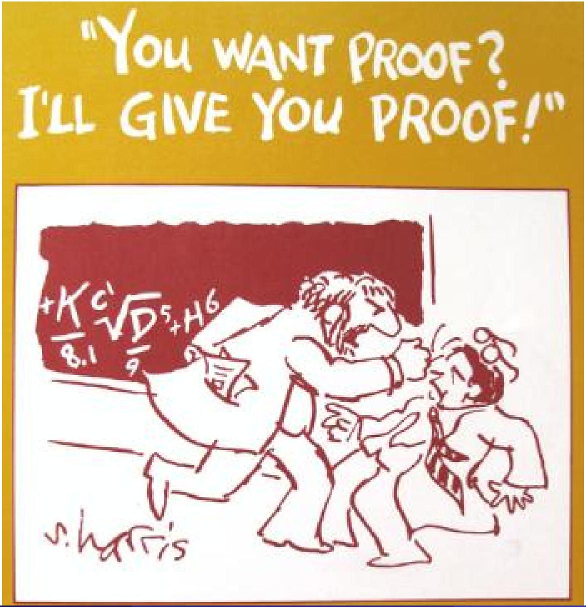
Conclusions

Why hydrodynamics?

- Interesting — involving modeling (PDE) of multi-physics and multi-scale problems;
- Useful — wide variety of applications;
- Challenging — many difficult problems remained solved.

Other Applications

- Ladd, Univ. Florida: Cluster of 1812 particles
- Flow through Porous Media (Krafczyk *et al.*, TUB):
  - Air through fluids in a packed-sphere bio-filter
  - Multi-component flow past porous media: imbibe, drain, re-imbibe
- Free-Surface Flow (Krafczyk *et al.*, TUB):
  - A single drop impact on a liquid surface
  - Flow coming down from a dam
  - Flow past through/over a bridge
  - Flow interacts with a column
- Droplet collision (Frohn *et al.*, Univ. Stuttgart):
  - Merge, Separate, and one extra; LBE vs. Experiment.
- More (Thüry *et al.*, Univ. Erlangen):
  - Bubbles rising in water tank
  - Metal foams


"YOU WANT PROOF?
I'LL GIVE YOU PROOF!"
s.harris