Čestični metodi za simulacije kompleksnih sistema

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Različiti pristupi u modelovanju

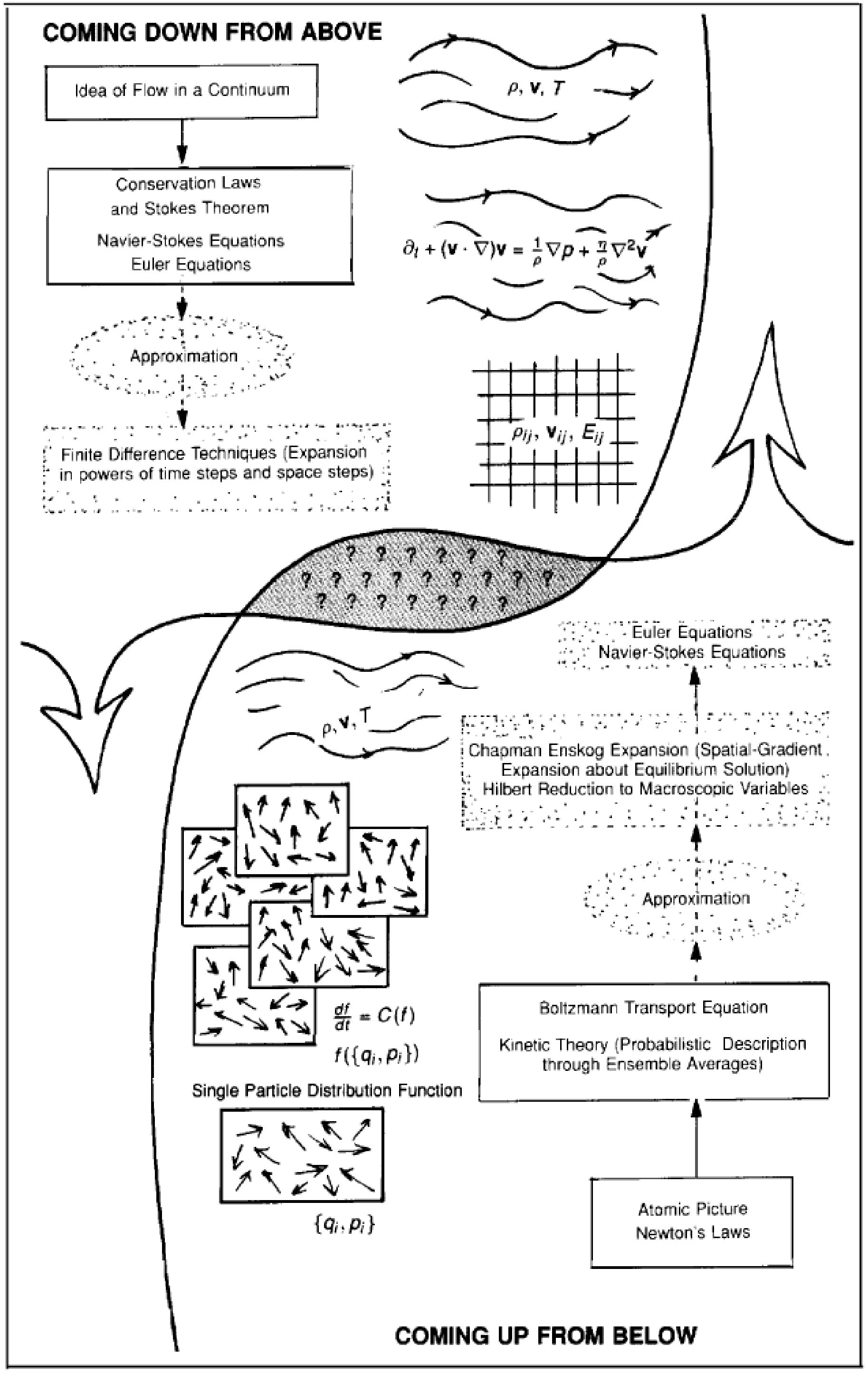


Fig. 2. Both the continuum view of fluids and the atomic picture lead to the Navier-Stokes equations but not without approximations (dashed lines). The text emphasizes how cellular-automaton models embody the essentials of both points of view.

Mehanika fluida - ukratko

Posmatrani element Σ mora biti dovoljno

(1) veliki da molekularna strukutra može da se zameni kontinualnim modelima

(2) dovoljno mali da bi bio matematički prihvatljiv

onda geometrijskih razmatranja + $\oint_{\partial\Sigma} \mathbf{A}\cdot\mathbf{d}l = \oint_{\Sigma} \nabla\times\mathbf{A}\cdot d\mathbf{S}$ & $\oint_{\partial\Sigma} \mathbf{A}\cdot d\mathbf{S} = \int_{\Sigma} \nabla\cdot\mathbf{A}\, dV$

dobija se:

$$\overbrace{\oint_{\partial\Sigma} \rho\,\mathbf{v}\cdot d\mathbf{S}}^{\text{flux of mass}} = -\partial_t \overbrace{\int_{\Sigma} \rho\, dV}^{\text{mass}} = \int_{\Sigma} \nabla\cdot(\rho\,\mathbf{v})\, dV \xrightarrow[\Sigma\to 0]{} \boxed{\partial_t\rho + \nabla\cdot(\rho\,\mathbf{v}) = 0}$$

jednačina kontinutieta

pritisak je sila na jedinicu zapremine

$$-\oint_{\partial\Sigma} p\, d\mathbf{S} = -\int_{\Sigma} \nabla p\, dV$$

$$\mathbf{F} = m\,\mathbf{a} = \int_{\Sigma} \rho \frac{d\mathbf{v}}{dt} dV$$

$$\xrightarrow[\Sigma\to 0]{} -\nabla p = \rho \frac{d\mathbf{v}}{dt} \longrightarrow \boxed{\partial_t\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p}$$

Eulerova jednačina

$$\boxed{\partial_t\mathbf{v} + (\mathbf{v}\cdot\nabla)\mathbf{v} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\mathbf{v}}$$

Navier-Stoksova jednačina

Mehanika fluida - ukratko

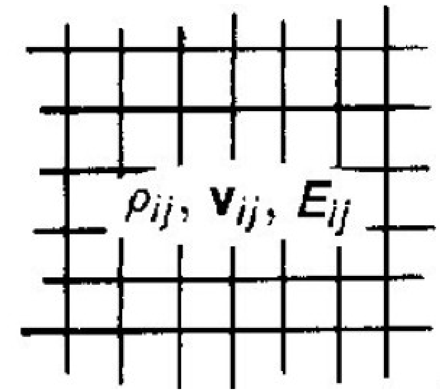
$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}$$

$$(\partial_t f)_{i,j}^n \approx \frac{f_{i,j}^{n+1} - f_{i,j}^n}{\Delta t}$$

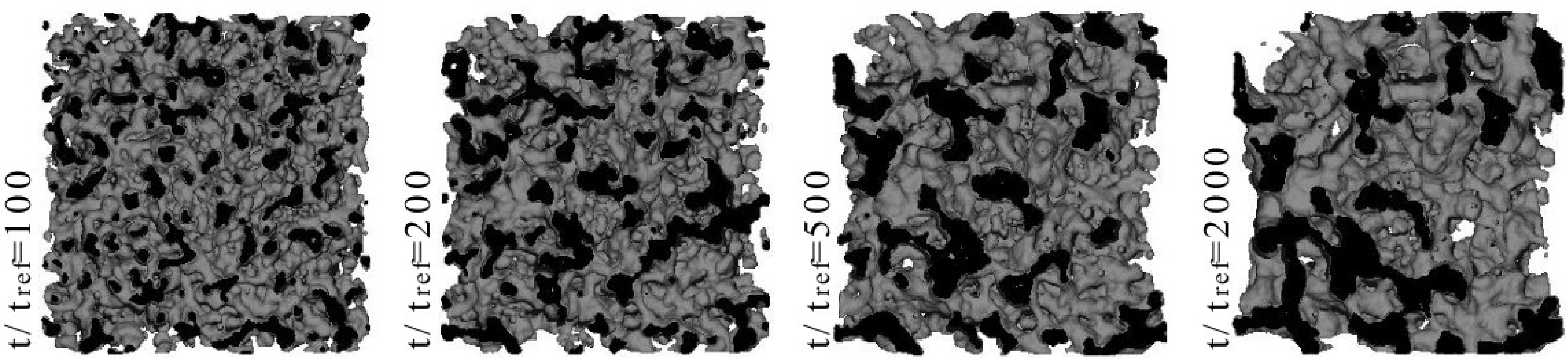
$$(\nabla_x f)_{i,j}^n \approx \frac{f_{i+1,j}^n - f_{i-1,j}^n}{\Delta x}$$

$$(\nabla_x^2 f)_{i,j}^n \approx \frac{f_{i+1,j}^n - 2 f_{i,j}^n + f_{i,j-1}^n}{2 \Delta x^2}$$



rešite diskretizovane numeričke jednačine na mreži tačaka

Šta ne može da reši mehanika fluida

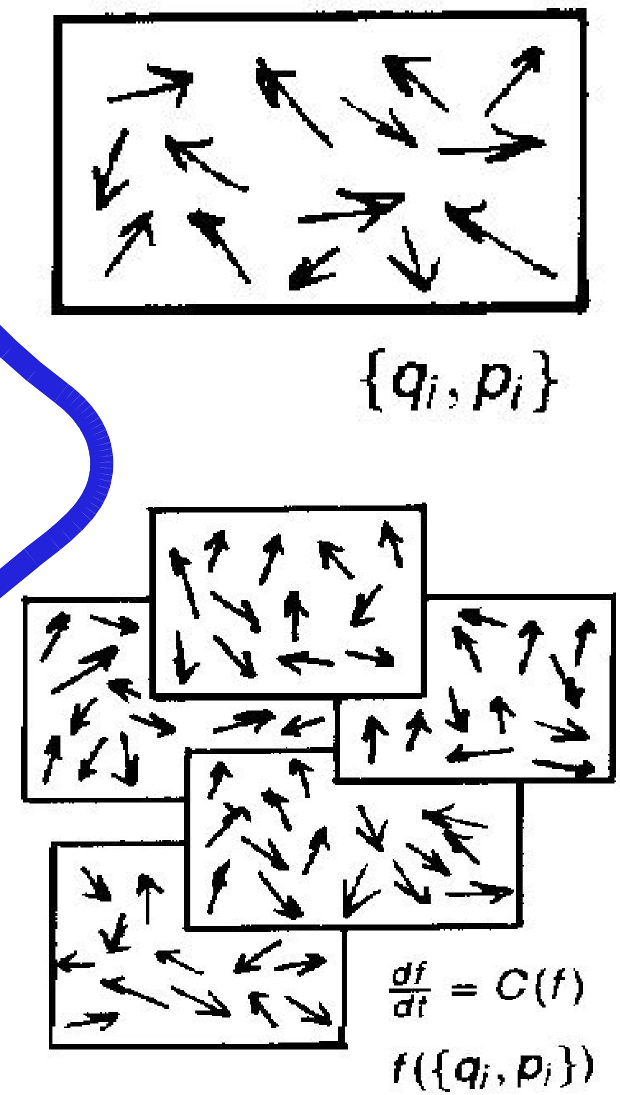


Pristup na malim skalama - ukratko

Čestice, atomi ili molekuli interaguju

preko klasičnih (ili kvantnih) potencijala

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$
$$\dot{\mathbf{v}}_i = -\nabla_i \mathbf{U}(\mathbf{r}_1, .., \mathbf{r}_N)$$



Single Particle Distribution Function

$$\langle n(\mathbf{r},t)\rangle = \int f(t,\mathbf{r},\mathbf{v})\, d\mathbf{v}$$
$$\langle \mathbf{V}(\mathbf{r},t)\rangle = (1/\langle n\rangle)\int f(t,\mathbf{r},\mathbf{v})\,\mathbf{v}\, d\mathbf{v}$$

srednje vrednosti iz jednočestične

funcije raspodele

Postoji li direktan prelaz iz kontinualnih u čestične modele

molekularni:

- **neravnotežna molekularna dinamika (NEMD)**
- Monte Karlo (MC)

mezoskopski methodi:

- Bolcmanovu jednačinu na rešetci (LB)
- braunovska dinamike (BD),
- disipativna čestična dinamika (DPD)

makroskopski metodi:

- **hidrodinamika ujednačenih čestica (SPH)**

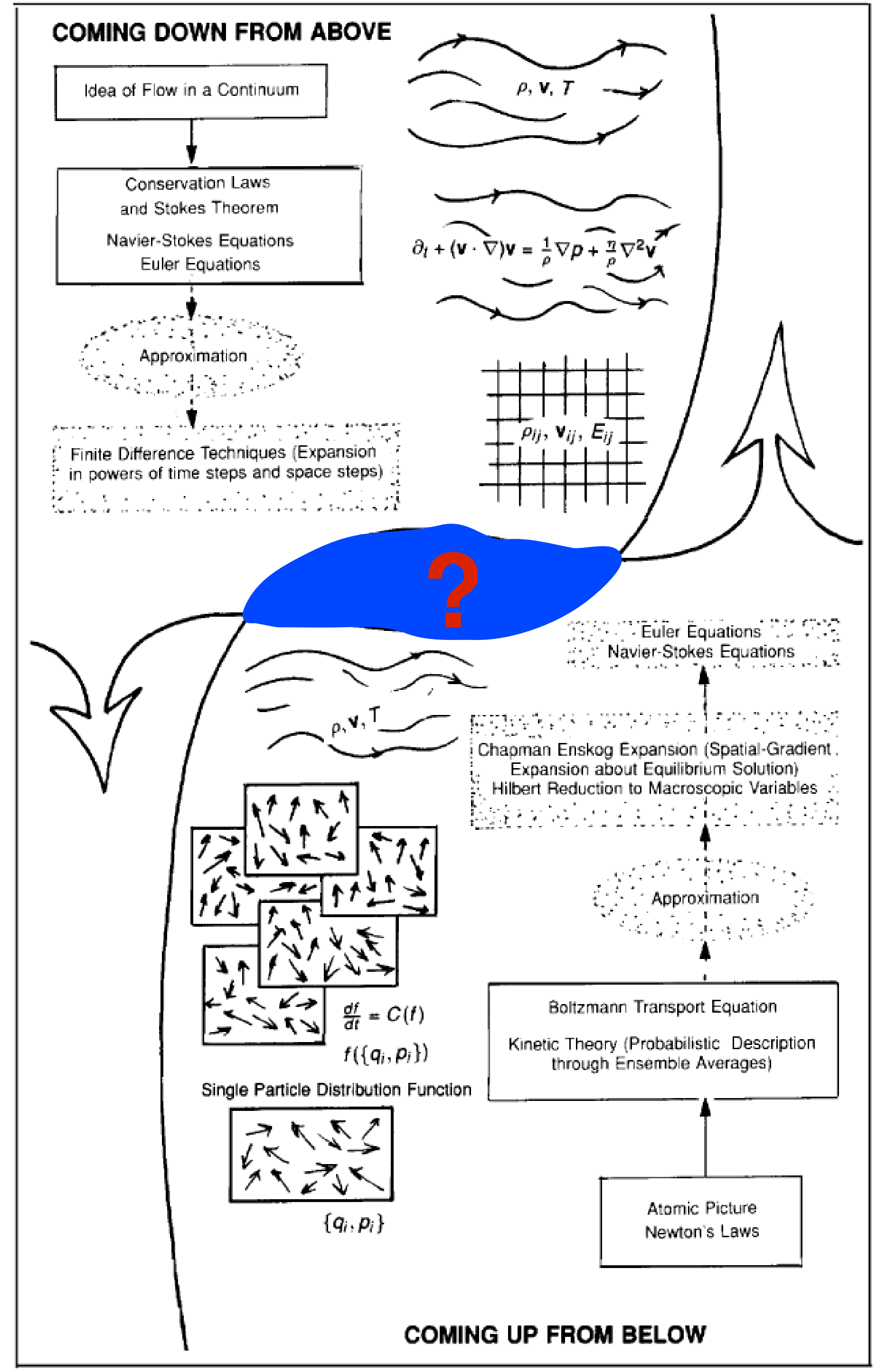


Fig. 2. Both the continuum view of fluids and the atomic picture lead to the Navier-Stokes equations but not without approximations (dashed lines). The text emphasizes how cellular-automaton models embody the essentials of both points of view.

Metod molekularne dinamike

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$
$$\dot{\mathbf{v}}_i = -\nabla_i V(\mathbf{r}_1, .., \mathbf{r}_N)$$

molekuli, atomi

$$V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \sum_i \sum_{j>i} \phi(|\mathbf{r}_i - \mathbf{r}_j|)$$

$$\phi_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

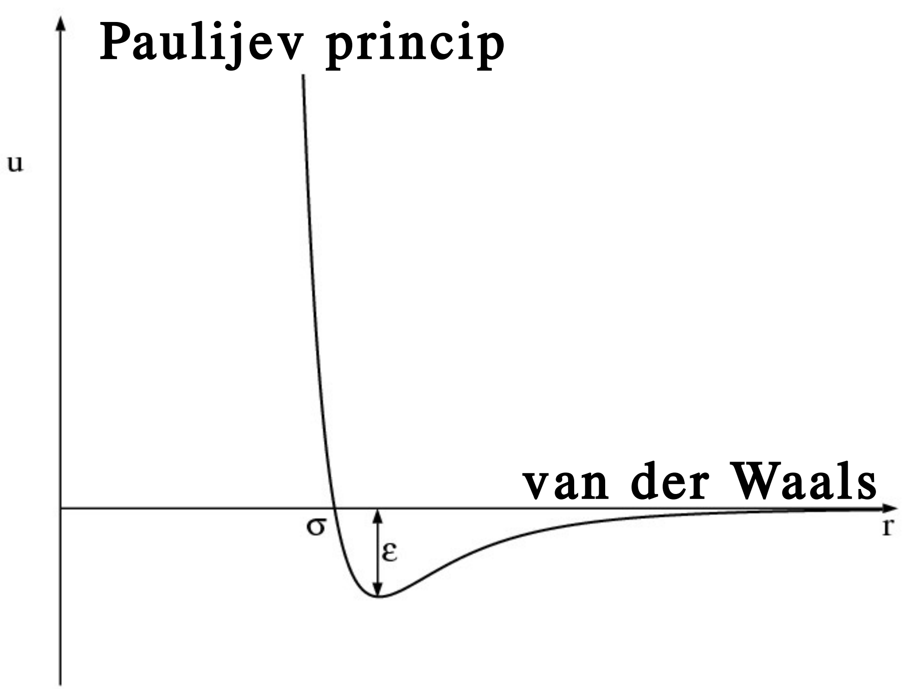
metali, poluprovodnici

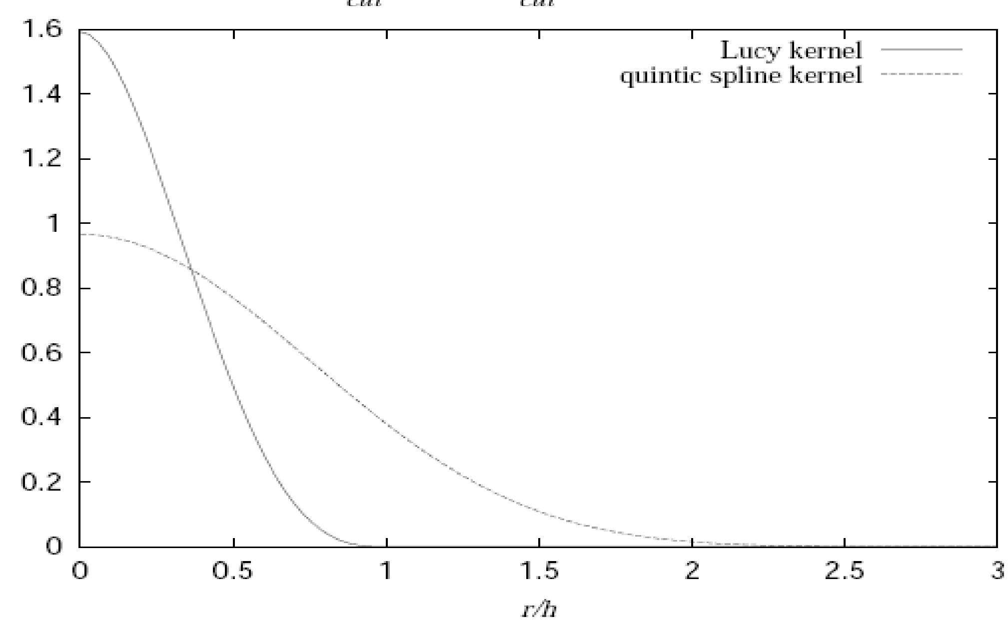
$$V(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \sum_i \left(\sum_{j>i} \phi(|\mathbf{r}_i - \mathbf{r}_j|) + \Theta(\rho_i)\right)$$

$$\Theta(\rho_i) = \phi_0 \sum_{k=2,4,\dots} r_0^3 k\, F_k((\rho_i - \rho_{des})^k - (w(0) - \rho_{des})^k)$$

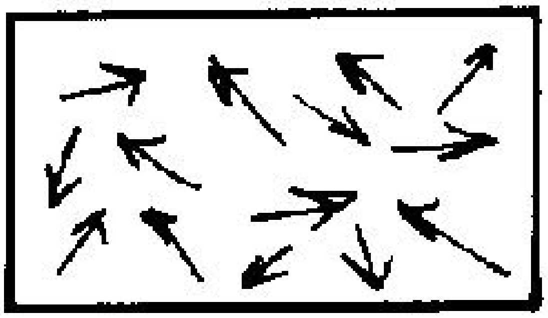
lokalna gustina

$$\rho_i = \sum_j w(r_{ij})$$
$$w(r) = w_0 (1 + 3\frac{r}{r_{cut}})(1 - \frac{r}{r_{cut}})^3$$





Metod molekularne dinamike



$\{q_i, p_i\}$

$V(t)=\sum_i \sum_{j>i} \phi(|\mathbf{r}_i(t)-\mathbf{r}_j(t)|)$ potencijalna energija

$K(t)=\frac{1}{2}\sum_i m_i[v_i(t)]^2$ kinetička energija

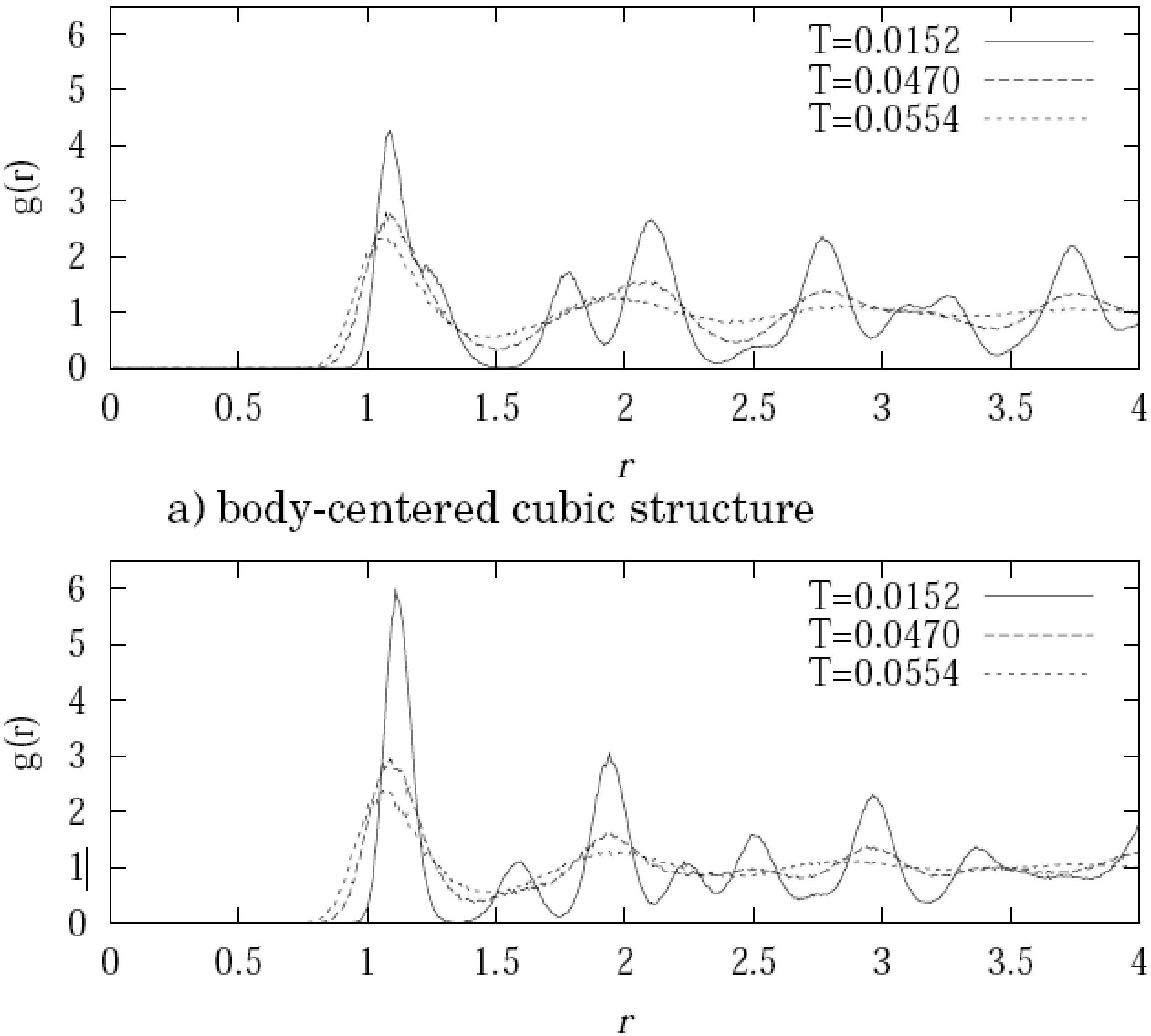
$E(t)=K(t)+V(t)$

$K(t)=\frac{3}{2}N k_B T(t)$ temperatura

$PV = N k_B T - \frac{1}{3}\langle \sum_i \mathbf{r}_i \cdot \mathbf{F}_i \rangle$ pritisak

$D=\lim_{t\to\infty} \frac{1}{6t}\langle |\mathbf{r}(t)-\mathbf{r}(0)|^2 \rangle$ koeficijent difuzije

Metod molekularne dinamike



a) body-centered cubic structure

b) face-centered cubic structure

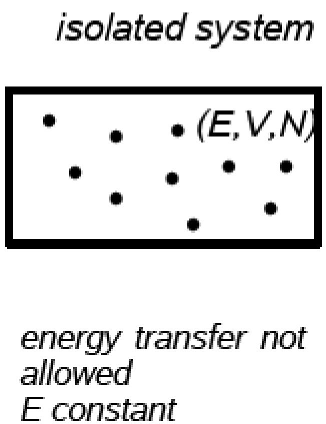
$$\rho\, g(r) = \frac{1}{N} \langle \sum_i \sum_{j \neq i} \delta(r - r_{ij}) \rangle$$

dvočestična funkcija

raspodele

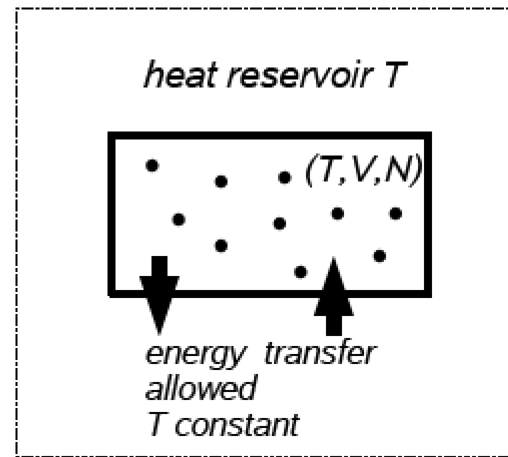
Metod molekularne dinamike

- *Microcanonical ensemble*



$$f(\Gamma)=\delta(H(\Gamma)-E)$$

- *Canonical ensemble*



$$f(\Gamma)=exp(-H(\Gamma)/k_B T)$$

potrebne su dodatne jednačine

Metod molekularne dinamike

Nose-Hoover termostat

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i}$$

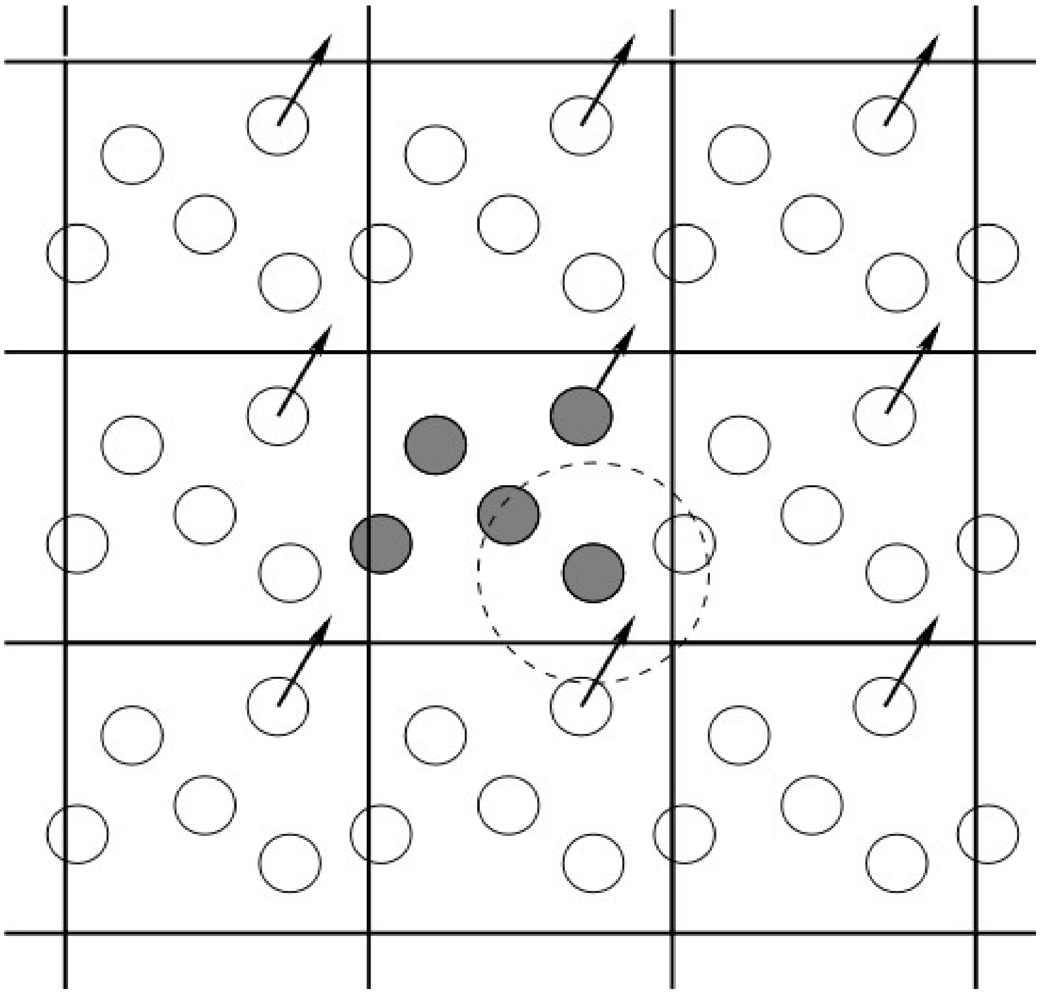
$$\dot{\mathbf{p}}_i = -\nabla_i V - \zeta \mathbf{p}_i$$

$$\dot{\zeta} = \frac{\left(\sum_i \frac{\mathbf{p}_i^2}{m_i} - g k_B T \right)}{Q} = \nu_T \left[\frac{\sum_i \frac{\mathbf{p}_i^2}{m_i}}{g k_B T} - 1 \right] = \nu_T \left[\frac{T^*}{T} - 1 \right]$$

Woodcock termostat

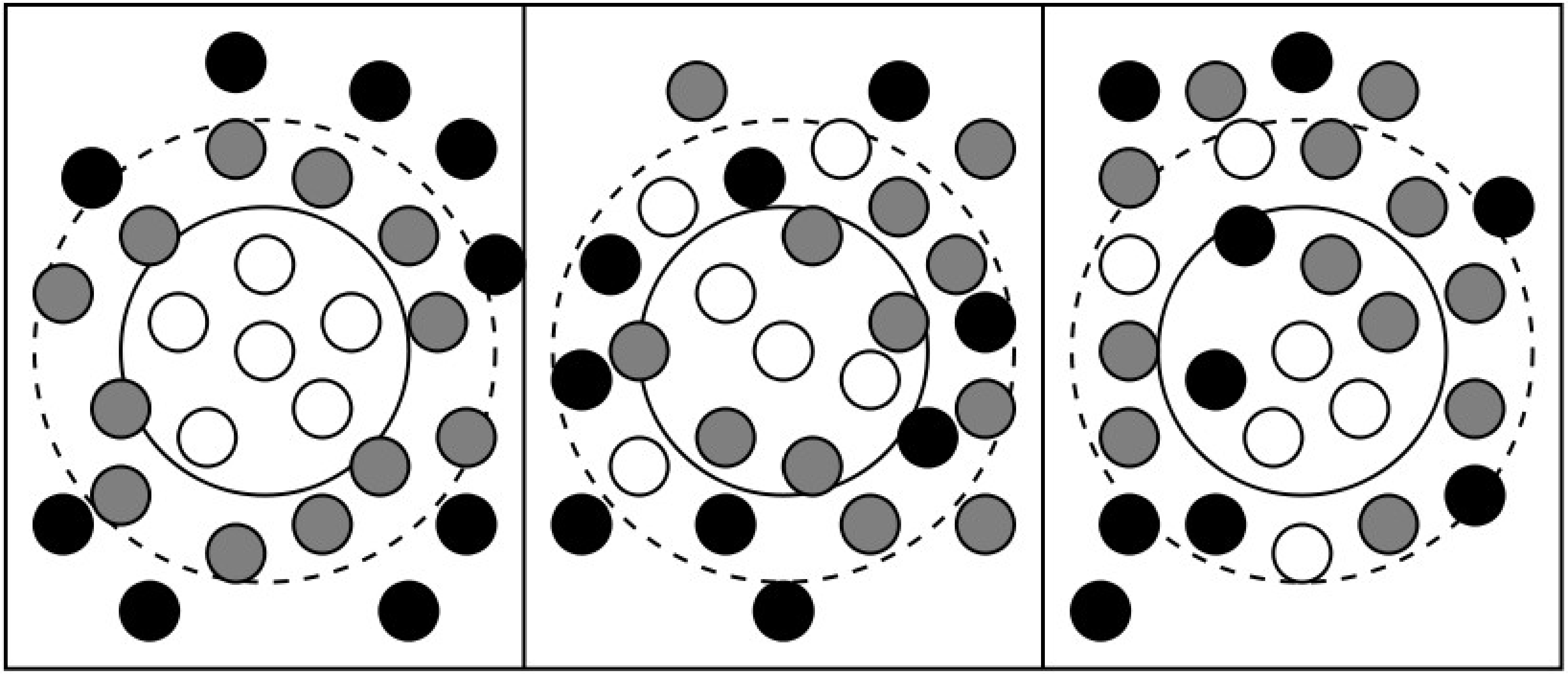
$$\hat{\mathbf{v}}_i \left(t + \frac{\Delta t}{2} \right) = S \mathbf{v}_i \left(t + \frac{\Delta t}{2} \right) \quad \Rightarrow \quad S = \left[\frac{\frac{3}{2} N k_B T}{\sum_i \frac{m_i}{2} \left[\mathbf{v}_i \left(t + \frac{\Delta t}{2} \right) \right]^2} \right]^{1/2}$$

Metod molekularne dinamike



periodični granični uslovi

Metod molekularne dinamike



liste suseda za smanjivanje kompleksnosti problema

Mehanika fluida - ukratko

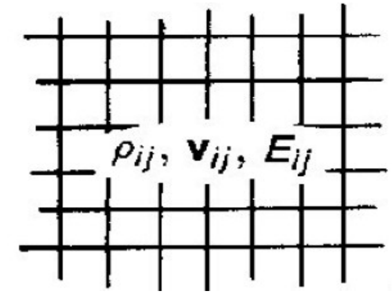
$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v}$$

$$(\partial_t f)^n_{i,j} \approx \frac{f^{n+1}_{i,j} - f^n_{i,j}}{\Delta t}$$

$$(\nabla_x f)^n_{i,j} \approx \frac{f^n_{i+1,j} - f^n_{i-1,j}}{\Delta x}$$

$$(\nabla^2_x f)^n_{i,j} \approx \frac{f^n_{i+1,j} - 2 f^n_{i,j} + f^n_{i,j-1}}{2 \Delta x^2}$$



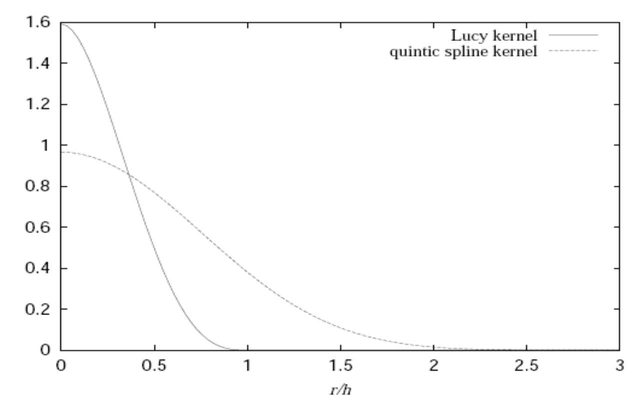
Hidrodinamika ujednačenih čestica (SPH)

$$\langle f(\mathbf{x}) \rangle = \int_\Omega f(\mathbf{x}') W(\mathbf{x} - \mathbf{x}', h)\, d\mathbf{x}'$$

$$\int_\Omega W(\mathbf{x} - \mathbf{x}', h) d\mathbf{x}' = 1,$$

$$\lim_{h \to 0} W(\mathbf{x} - \mathbf{x}', h) = \delta(\mathbf{x} - \mathbf{x}')$$

$$n(\mathbf{x}) = \sum_j \delta(\mathbf{x} - \mathbf{x}_j)$$



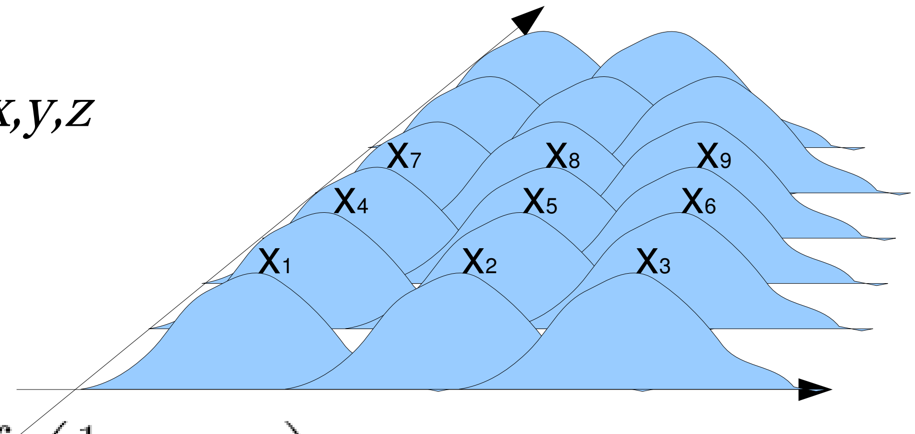
dx je zamenjen zapreminom čestice

$$d\mathbf{x}' \to \phi_j \equiv \frac{m_j}{\rho_j}$$

Hidrodinamika ujednačenih čestica (SPH)

$$\frac{\partial V^{\alpha}}{\partial t} + (V^{\beta}\nabla^{\beta})V^{\alpha} = \frac{1}{\rho}\nabla^{\beta}P^{\alpha\beta}$$

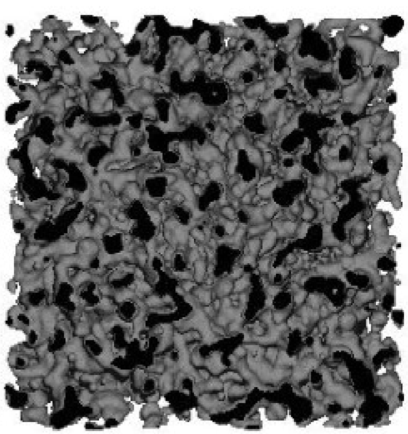
$\alpha,\beta = x,y,z$



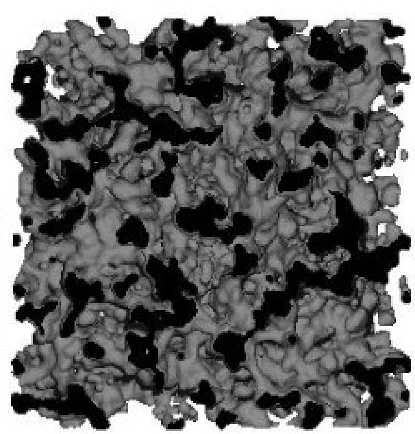
$$\int_{\Omega}\left(\frac{\partial V^{\alpha}}{\partial t} + (V^{\beta}\nabla'^{\beta})V^{\alpha}\right)W(|\mathbf{x}-\mathbf{x}'|,h)\,d\mathbf{x}' = \int_{\Omega}\left(\frac{1}{\rho}\nabla'^{\beta}P^{\alpha\beta}\right)W(|\mathbf{x}-\mathbf{x}'|,h)\,d\mathbf{x}'$$

$$\frac{dV_i^{\alpha}}{dt} = \sum_j m_j \boxed{\left(\frac{P_i^{\alpha\beta}}{\rho_i^2} + \frac{P_j^{\alpha\beta}}{\rho_j^2}\right)} \nabla_i^{\alpha}W_{ij}$$

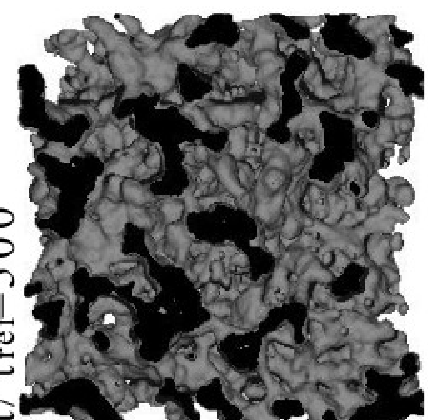
$t/t_{ref}=100$



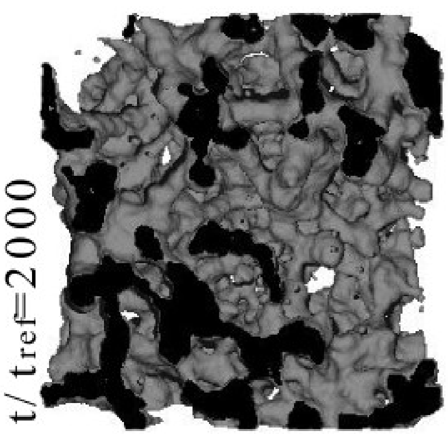
$t/t_{ref}=200$



$t/t_{ref}=500$

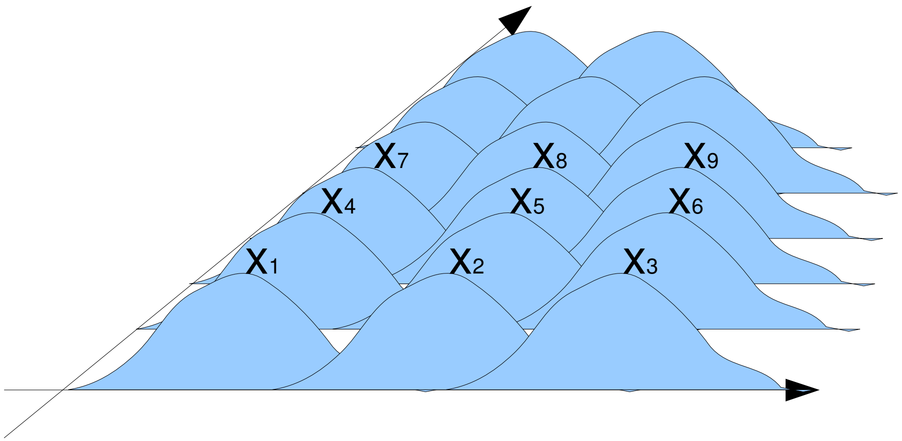


$t/t_{ref}=2000$



Hidrodinamika ujednačenih čestica (SPH)

$$\frac{dV_i^\alpha}{dt} = \sum_j m_j \boxed{\left(\frac{P_i^{\alpha\beta}}{\rho_i^2} + \frac{P_j^{\alpha\beta}}{\rho_j^2}\right)} \nabla_i^\alpha W_{ij}$$



$P \sim \rho^2$

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$\dot{\mathbf{v}}_i = -\nabla_i V(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

Kako integrisati dve skale?

$$\frac{dV_i^\alpha}{dt} = \sum_j m_j \left(\frac{P_i^{\alpha\beta}}{\rho_i^2} + \frac{P_j^{\alpha\beta}}{\rho_j^2} \right) \nabla_i^\alpha W_{ij}$$

inerpretacija

čestice

pritisak

površinski napon

termostat

$$\dot{\mathbf{r}}_i = \mathbf{v}_i$$

$$\dot{\mathbf{v}}_i = -\nabla_i V(\mathbf{r}_1, .., \mathbf{r}_N)$$

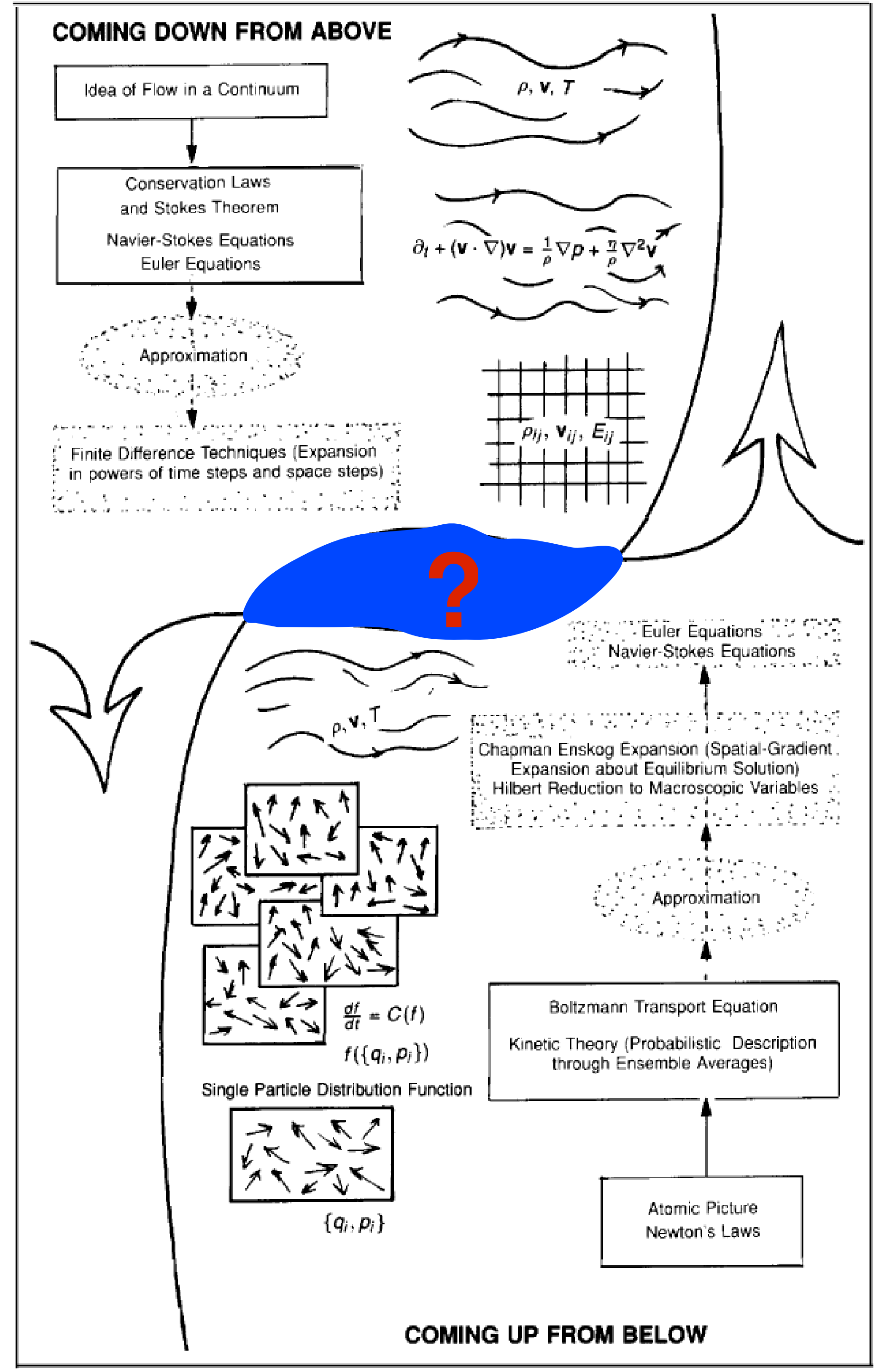
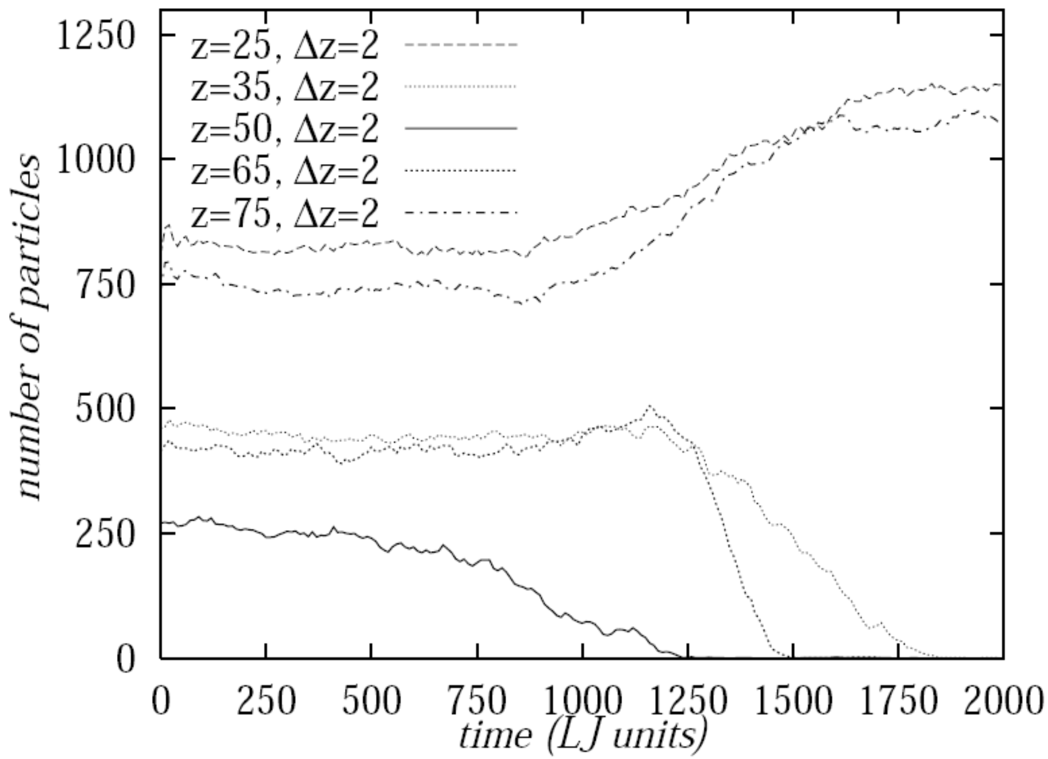
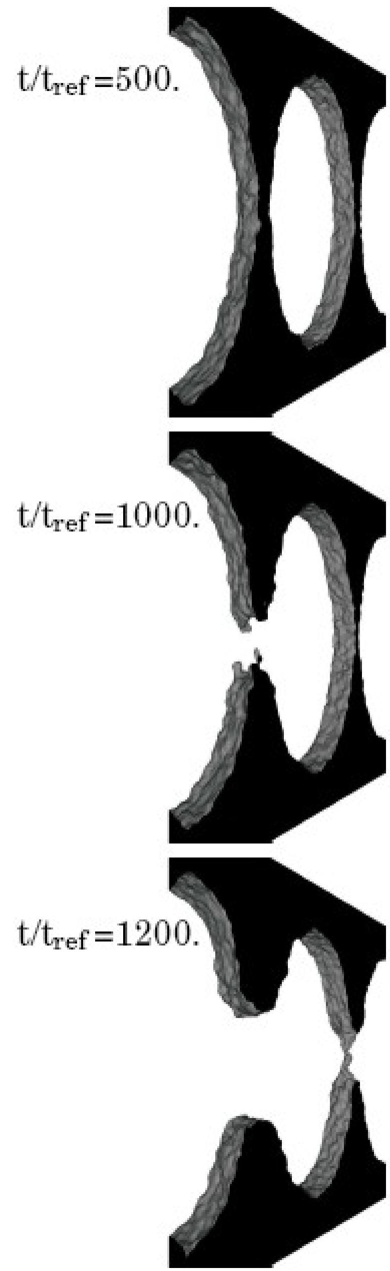
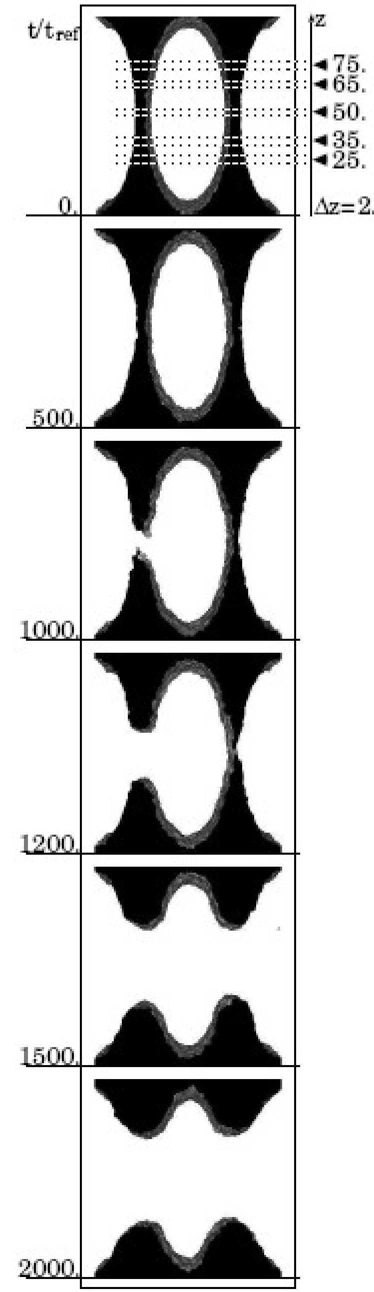


Fig. 2. Both the continuum view of fluids and the atomic picture lead to the Navier-Stokes equations but not without approximations (dashed lines). The text emphasizes how cellular-automaton models embody the essentials of both points of view.

Kako integrisati dve skale?







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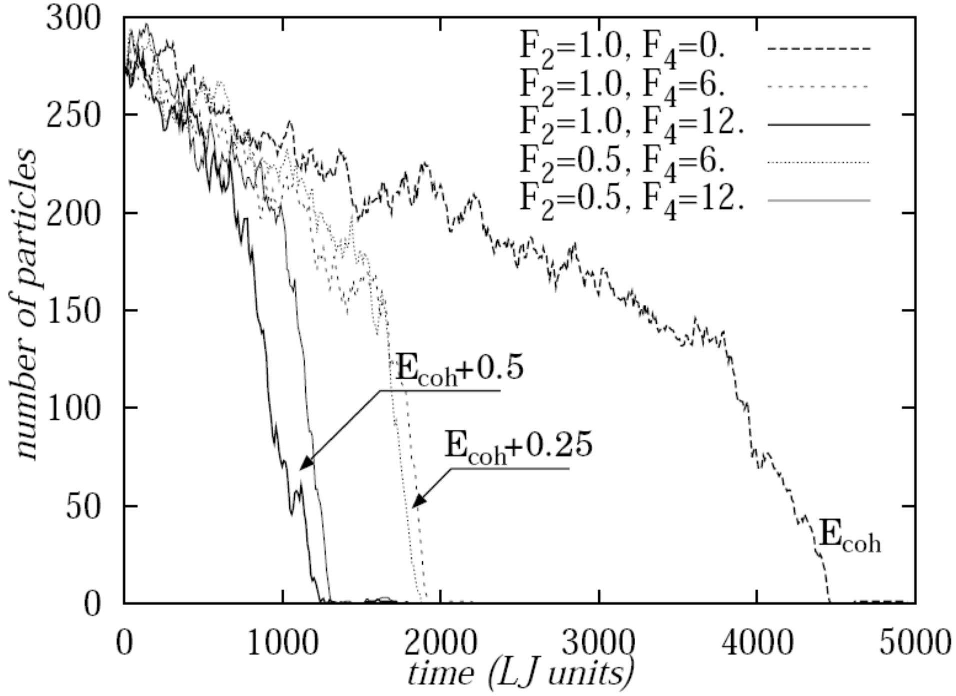

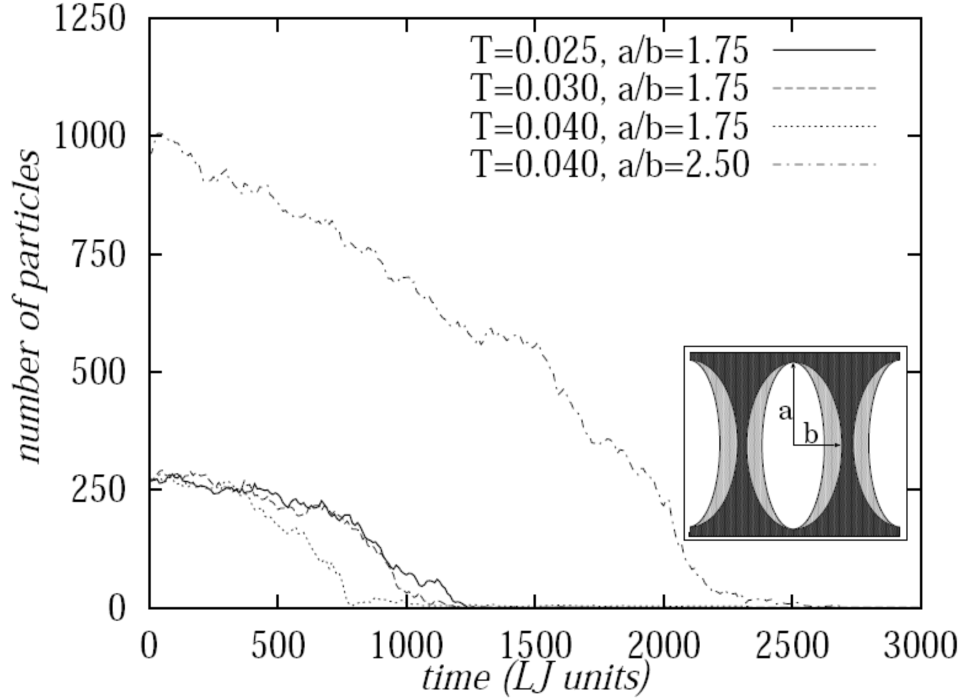

system (atoms)	$r_{\rm ref}$ (nm)	$E_{\rm ref}, k_{\rm B}T$	$\Gamma_{\rm ref}$ (erg/cm^2)	$P_{\rm ref}$	$t_{\rm ref}$
embedded atoms	0.24	3.45eV, 40kK	0.96		0.97×10^{-13}s
(8)	0.48	27.6eV	1.92		1.9×10^{-13}s
embedded (64)	0.96	0.2keV	3.83	40GPa	3.9×10^{-13}s
particles (500)	1.92	1.8keV	7.67		7.8×10^{-13}s
(4000)	3.84	14keV	15.3		0.97×10^{-12}s