Large Scale High Resolution Blood Flow Simulations

Florian Janoschek* Jens Harting*† Federico Toschi*‡

*Department of Applied Physics, Eindhoven University of Technology, The Netherlands
†Institute for Computational Physics, Stuttgart University, Germany
‡Department of Mathematics and Computer Science, Eindhoven University of Technology, The Netherlands and CNR-IAC, Rome, Italy

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Human blood

- Composition
  - $\approx 55$ vol. % plasma
  - $\approx 44$ vol. % red blood cells (RBCs): deformable biconcave discs
  - $< 1$ vol. % white blood cells, platelets, ...
- Non-Newtonian behavior: shear thinning
Length scales
- cell diameter $\sim 8 \mu m$
- vessel diameters
  $\sim 5 \mu m$ (capillaries) to
  $\sim 1 \text{ cm}$ (arteries)

artwork: www.prelabs.com
Mesoscopic blood model

Hydrodynamic long range interactions

- lattice Boltzmann method (D3Q19, BGK)
- ellipsoidal rigid particles [Ladd/Aidun]

Empirical short range interactions

- no lubrication corrections
- repulsive spring potential $\phi(r_{ij}) = \begin{cases} \varepsilon \left( \frac{1}{r_{ij}} - \frac{1}{\sigma} \right)^2 & r_{ij} < \sigma \\ 0 & r_{ij} \geq \sigma \end{cases}$

- orientation-dependent energy and range parameters $\varepsilon(\hat{o}_i, \hat{o}_j)$ and $\sigma(\hat{o}_i, \hat{o}_j, \hat{r}_{ij})$ [Berne and Pechukas]

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Empirical short range interactions

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  \[ \phi(r_{ij}) = \begin{cases} 
  \varepsilon \left(1 - \frac{r_{ij}}{\sigma}\right)^2 & r_{ij} < \sigma \\
  0 & r_{ij} \geq \sigma 
\end{cases} \]
- orientation-dependent energy and range parameters \( \varepsilon(\hat{o}_i, \hat{o}_j) \) and \( \sigma(\hat{o}_i, \hat{o}_j, \hat{r}_{ij}) \) [Berne and Pechukas]
Good scalability due to high degree of *locality*

- collision

\[ n_r^*(x, t) = n_r(x, t) - \Omega(x, t) \]

- advection

\[ n_r(x + c_r, t + 1) = n_r^*(x, t) \]
Lattice Boltzmann method

Good scalability due to high degree of *locality*

- **collision**
  \[ n_r^*(x, t) = n_r(x, t) - \Omega(x, t) \]

- **advection**
  \[ n_r(x + c_r, t + 1) = n_r^*(x, t) \]

- **spatial decomposition** easily applicable
Application to different problems

Determination of model parameters

Unsteady flow in microvasculature

Fåhræus-Lindqvist

Blood in Motion

- DECI-5 project
- HUYGENS (IBM power6, SARA)
  HECToR (Cray XT4/XE6, EPCC)
  Louhi (Cray XT4/5, CSC)
- 4M core hours
- 2010-01–2010-09

Further parameter studies
Channel flow
Cell statistics
Apparent blood viscosity

untreated blood

viscosity $\mu_{\text{app}}/\mu_{\text{plasma}}$

shear rate $\dot{\gamma} [\text{s}^{-1}]$

$10^0$ $10^1$ $10^2$ $10^3$

$10^{-2}$ $10^{-1}$ $10^0$ $10^1$ $10^2$ $10^3$

Chien, 1970

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Apparent blood viscosity

\[ \frac{\mu_{\text{app}}}{\mu_{\text{plasma}}} \]

shear rate \( \dot{\gamma} \) [s\(^{-1}\)]

untreated blood
no cell aggregation

data [Chien, 1970]

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Apparent blood viscosity

\[ \frac{\mu_{\text{app}}}{\mu_{\text{plasma}}} \]

- untreated blood
- no cell aggregation
- no cell deformation

Data [Chien, 1970]
Apparent blood viscosity

Comparison for region of high shear rates

» Experiment

σ

\[ \frac{\mu_{\text{app}}}{\mu_{\text{plasma}}} \]

\[ \dot{\gamma} \ [s^{-1}] \]

deformation

no △

yes □

data [Chien, 1970]

» Simulation

σ

\[ \frac{\mu_{\text{app}}}{\mu_{\text{plasma}}} \]

\[ \dot{\gamma} \ [s^{-1}] \]

cell stiffness

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Kolmogorov flow

- sinusoidally modulated volume force

\[ f(x) = f_0 \sin(kx) \]

- spatial variation of shear stress \( \sigma \)

\[ \partial_x \sigma(x) = f(x) \]

[Benzi et al., 2010]

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Kolmogorov flow

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  \[ f(x) = f_0 \sin(kx) \]

- spatial variation of shear stress \( \sigma \)
  
  \[ \partial_x \sigma(x) = f(x) \]

- integration yields
  
  \[ \sigma(x) = -\frac{f_0}{k} \cos(kx) \]

[Benzi et al., 2010]

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Kolmogorov flow

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- integration yields
  \[ \sigma(x) = -\frac{f_0}{k} \cos(kx) \]

- local shear rate
  \[ \dot{\gamma}(x) = \partial_x u_z(x) \]

[Benzi et al., 2010]
Results

\[ k = \frac{2\pi}{(85 \mu m)}, \quad f_0 = 1.49 \times 10^5 \text{ N/m}^3 \]

- periodic boundary conditions; no boundary effects
- results for several shear rates from one simulation run


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Results

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F. Janoschek, F. Mancini, J. Harting, and F. Toschi. Phil. Trans. R. Soc. London A, in press; 


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Results

- periodic boundary conditions; no boundary effects
- results for several shear rates from one simulation run
- consistency with data obtained from Couette flow

F. Janoschek, F. Mancini, J. Harting, and F. Toschi. Phil. Trans. R. Soc. London A, in press; 


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Tumbling of a single ellipsoidal particle

Analytical solution [Jeffery, 1922]

\[ T^* = \frac{\pi (R^2_\perp + R^2_\parallel)}{\dot{\gamma} R_\perp R_\parallel} \]
Tumbling of many soft particles I

\[ T \alpha_{\pi} \]

\[ \alpha \]
most frequent period $T$ close to single particle value $T^*$ [Jeffery, 1922]

Tumbling of many soft particles II

- most frequent period $T$ close to single particle value $T^*$ [Jeffery, 1922]
- for high volume concentrations $\Phi$ broad distributions with a long tail at large tumbling periods $T$

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-for high volume concentrations $\Phi$ broad distributions with a long tail at large tumbling periods $T$

JUGENE (IBM BG/P, JSC)
397 rack days
2010-11–2011-10

...in Realistic Vessel Geometries

revise model
improve statistics
IBM BlueGene/P at JSC: JUGENE

- compute node
  - quadcore CPU, 850 MHz
  - 2 GB RAM
- 73,728 compute nodes
  - 294,912 CPU cores in total
- 3D torus network

photo: FZ Jülich
Matching network topology

The graph shows the normalized speedup $\tilde{S}$ as a function of the number of cores $P$ for 1024 lattice sites. The speedup is plotted before and after optimization.

1 Newtonian fluid component,
$1024^2 \times 2048$ lattice sites
BlueGene/P Extreme Scaling Workshop

- Matching network topology
- Reducing serial code fraction

![Graph showing normalized speedup vs. number of cores](image)

1 Newtonian fluid component, $1024^2 \times 2048$ lattice sites

Pickering emulsion: 2 fluid species + suspended particles

Matching network topology

Reducing serial code fraction

1 Newtonian fluid component, $1024^2 \times 2048$ lattice sites

Pickering emulsion: 2 fluid species + suspended particles
Effect of cells on the flow past an obstacle

- model for pathological stenoses in blood vessels
- shear stress affects both blood and endothelial cells
  - thrombus formation
  - further growth of the stenosis
Effect of cells on the flow past an obstacle

- periodic boundary conditions might bias our results
- cell configuration at inlet is not known a priori
Effect of cells on the flow past an obstacle

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Conclusions and outlook

- **Mesoscopic blood model** that bridges the gap between continuum models and high-resolution cell-based models
- **DEISA DECI-5** grant 2010-01–2010-09
- **PRACE** grant 2010-11–2011-10, ongoing work...
  - flow past obstacle
  - model for cell aggregation and membrane motion (tank-treading)
Bibliography I


