tP-CKM: Time-parallel continuum-kinetic-microscopic computation of non-equilibrated phenomena

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tP-CKM

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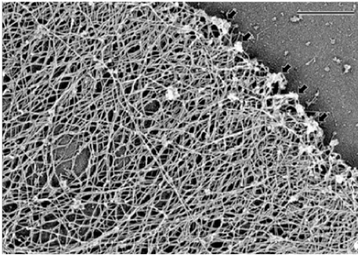
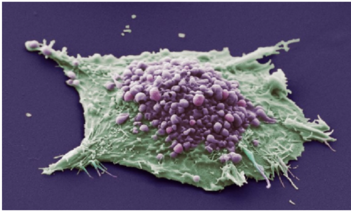
1. Paradigm
   - Typical problems
   - Goals
2. Approach
3. C $\leftrightarrow$ K
4. K $\leftrightarrow$ M
5. Results

Cytoskeleton

- Undergoes continuous reconfiguration
  - Actin filaments polymerize/depolymerize
  - Cross-links form/rupture
  - Membrane adhesion complexes form/rupture
- Biological functions
  - movement
  - triggers apoptosis (cellular death)
  - cancer metastasis





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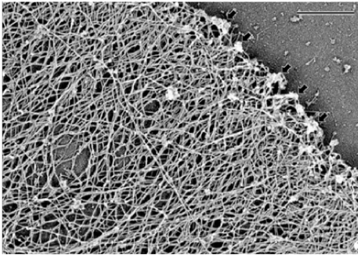
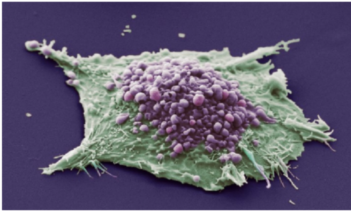
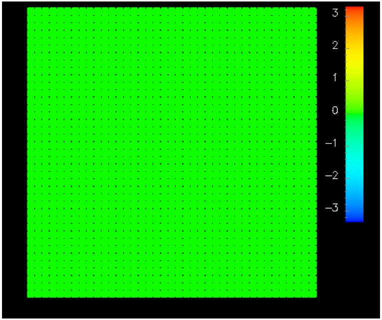




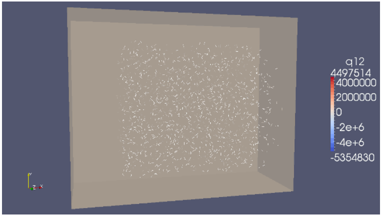
Maxwell equations in dispersive media

- Variety of relaxation times of electronic state
- Frequency dependent permittivity, permeability
- Maxwell system extended with equation(s) to track relaxation



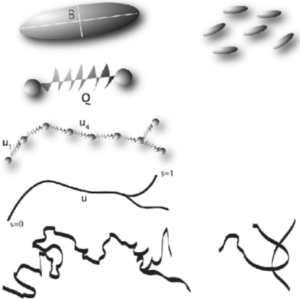
Crack propagation and fracture

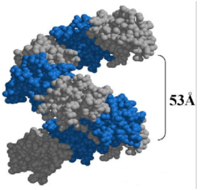
- Stress field imposed by boundary forces
- Local stress depends on instantaneous microconfiguration
- Microconfiguration changes dynamically



Polymer flows

- Macromolecule solutions in small-molecule solvent
- Inherently multiscale
- Hierarchy of models
    - Ellipsoids
    - Elastic dumbbells
    - Rouse beads
    - Kramer rods
    - Molecular dynamics





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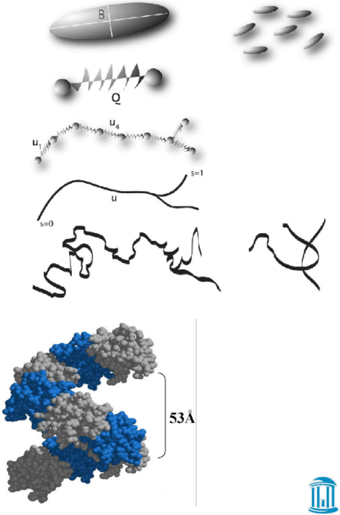

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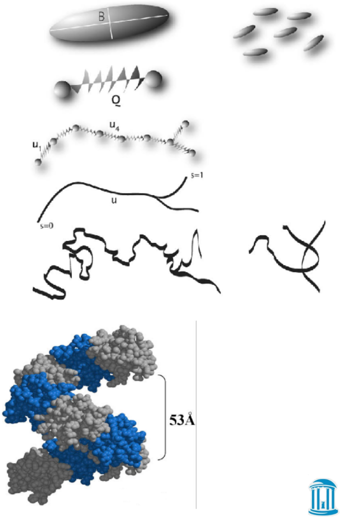
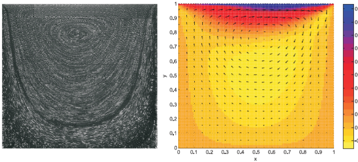


Polymer continuum models

- Conservation of mass

$$\nabla \cdot U = 0$$



$We = 0.15$

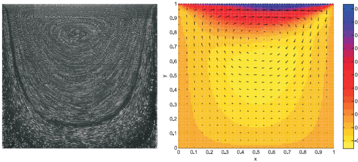
- Conservation of momentum

$$\partial_t U + (U \cdot \nabla)U = -\nabla P + \eta_s \nabla^2 U + \nabla \cdot \mathbf{T}$$

- Additional viscoelastic stress

$$\mathbf{T}(x,t) = \int \kappa(x,t,q)\psi(x,t,q)\mathrm{d}\mu(q)$$

Polymer continuum models



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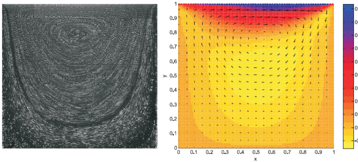

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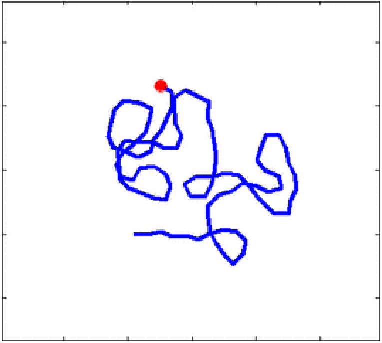
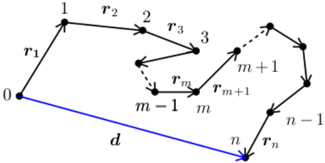
Polymer chain stochastic motion

- Intrinsic time scales
- Interaction between intrinsic and imposed time scales
- In general the flow is history dependent
- Exact analytical closures possible only for simplest models



Polymer models

- Microconfiguration
  $q(t) = (r_1(t), r_2(t), \ldots, r_n(t))$



- Microscopic: Langevin dynamics

$$\mathrm{d}q = \frac{\partial\phi}{\partial q}\mathrm{d}t + \sigma \mathrm{d}g(t)$$

- Kinetic: Fokker-Planck

$$\frac{\partial\psi}{\partial t} + \frac{\partial}{\partial q}\cdot\left(\frac{1}{\gamma}\frac{\partial\phi}{\partial q}\psi\right) = \frac{2k_B T}{\gamma}\frac{\partial}{\partial q}\cdot\frac{\partial\psi}{\partial q}$$

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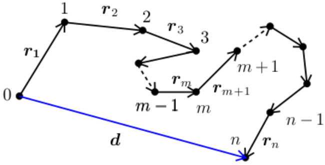

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Polymer models

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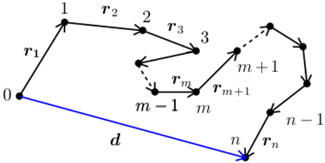
  $q(t) = (r_1(t), r_2(t), ..., r_n(t))$
- Microscopic: Langevin dynamics

$$dq = \frac{\partial \phi}{\partial q} dt + \sigma dg(t)$$



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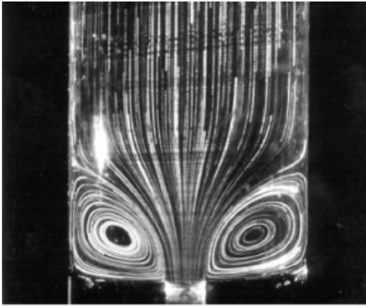
Kramers closure for dumbbell model → Oldroyd-B



- Viscoelastic stress is average of work done in deforming dumbbell springs

$$\tau = -nk_B TI + n\langle f(r)r\rangle$$

- Oldroyd-B viscoelastic stress evolution equation

$$\partial_t \mathbf{T} + U\cdot\nabla\mathbf{T} - (\nabla U)\mathbf{T} - \mathbf{T}(\nabla U)^T = -\mathbf{T}/\lambda + \eta_p(\nabla U + (\nabla U)^T)$$

- Model fails at high $We = \lambda\dot{\gamma}$

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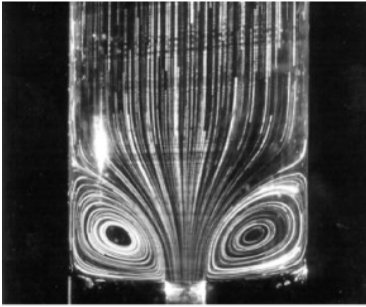

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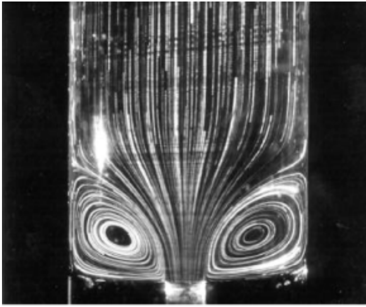

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Other constitutive models

- Oldroyd-B

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- FENE-P

$$\partial_t \mathbf{T} + U \cdot \nabla \mathbf{T} - (\nabla U)\mathbf{T} - \mathbf{T}(\nabla U)^T = -\mathbf{T}/\lambda - \frac{4H/\zeta}{1 - \mathrm{tr}(\mathbf{T})/q_0^2}\mathbf{T}$$

- Questions
  - Which model to choose?
  - With what confidence interval?
  - Are simple models useful?

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Solve a generic problem

- The continuum scale is of interest and is computable from microconfiguration
- Microconfiguration changes in response to continuum boundary conditions
- Physics specified at microscale
- Microscale is stochastic and does not equilibrate quickly

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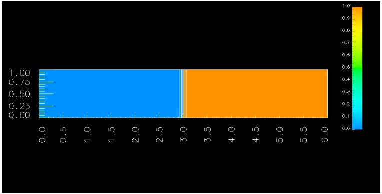
Software environment for multiscale problems

- BEARCLAW (Fortran, large runs))
  - multiphysics
  - adaptive mesh refinement
  - multiple levels of parallelism (MPI, OpenMPI, GPU threads)
- GPU execution
  - Fastest 6-core CPU: 30 GFlops
  - Tesla C2050 GPU: 600 GFlops
- Diapason (Python, prototyping)

`mitran-lab.amath.unc.edu:8084/redmine/projects`



tP-CKM

1. Paradigm

2. Approach
   - Overview
   - Parareal
   - Information flow

3. C ↔ K

4. K ↔ M

5. Results

Multiscale, multiphysics predictor-corrector

- Predict using continuum scale
  - Hypothesis: continuum model C is true, $P(C) = 1$
- Verify using microdynamics
  - In principle one could use $P(C|M) \propto P(M|C)P(C)$
  - Expensive: continuum priors on M insufficient for rapid Monte Carlo variance reduction
- Kinetic level as bridge
  - $P(C|K,M) \propto P(K|M,C)P(C)$
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  - second-order finite volume

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Parareal algorithm for ODEs $\dot{Q} = f(Q(t))$

- Use P available processors to reduce wall-clock computation time
- Solve on $[0, t_P]$, introduce subintervals
  - $[t_{j-1}, t_j]$, $j = 1, 2, \ldots, P$
  - $t_j = j\Delta t$, $\Delta t = t_P / P$
- Two ODE integrators
  - $K(t_{j+1}, t_j, Q_j^k)$ less accurate, cheap
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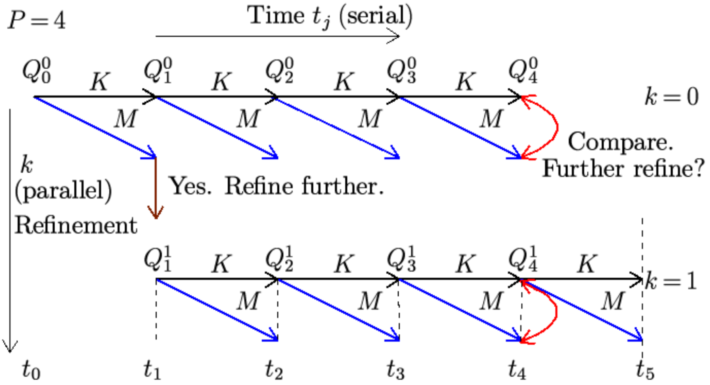
Parareal information flow

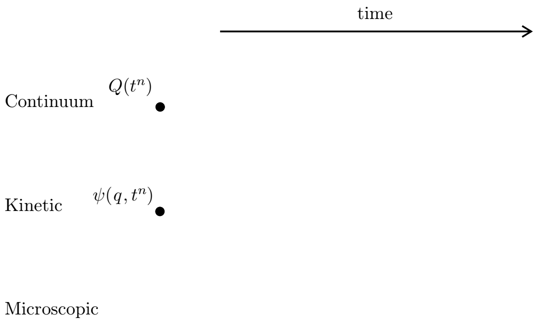
- Iterative update

$$Q_{j+1}^{k+1} = K(t_{j+1}, t_j, Q_j^{k+1}) + M(t_{j+1}, t_j, Q_j^k) - M(t_{j+1}, t_j, Q_j^{k+1})$$



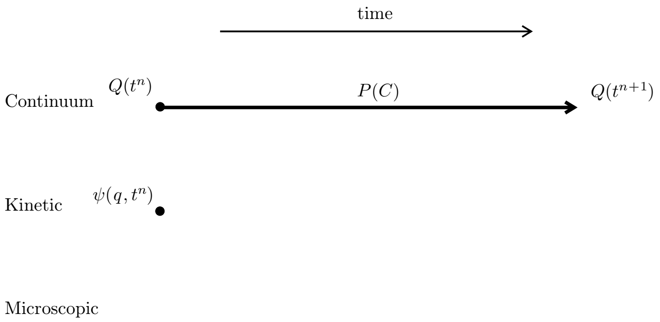
Initial state

- Known continuum, phase space states



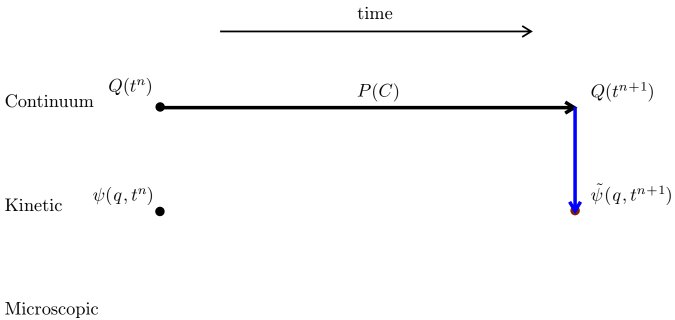
Continuum-level time evolution

- Continuum predictor



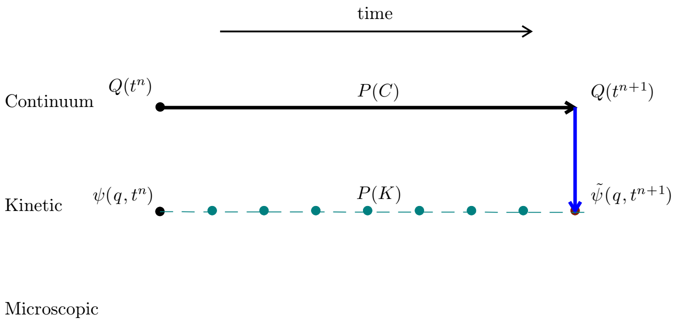
Impose continuum constraints on microconfiguration

- Modify previous probability density



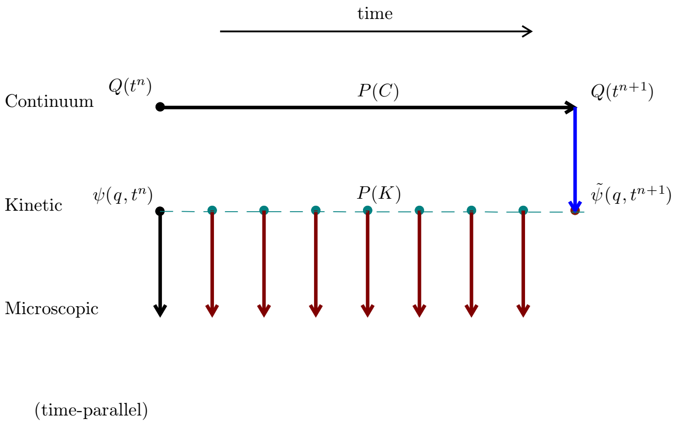
Kinetic-level time evolution

- Generate intermediate probability densities



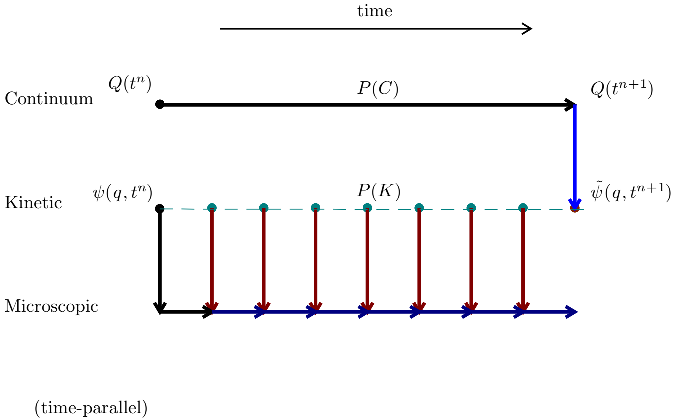
Instantiate microscopic scale

- Generate microscopic ensembles



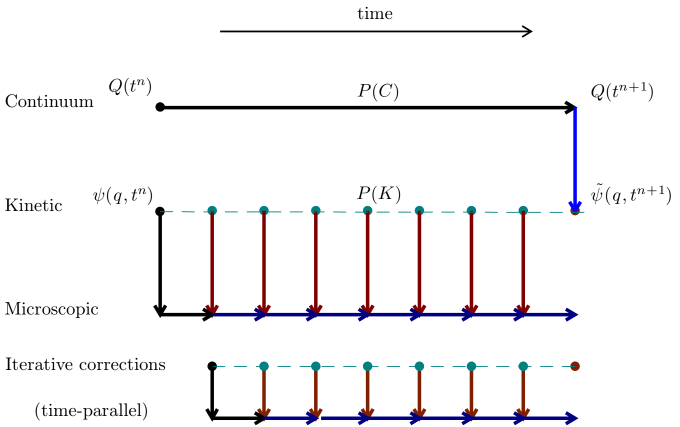
Microscopic-level time evolution

- Evolve stochastic differential equations (GPU)



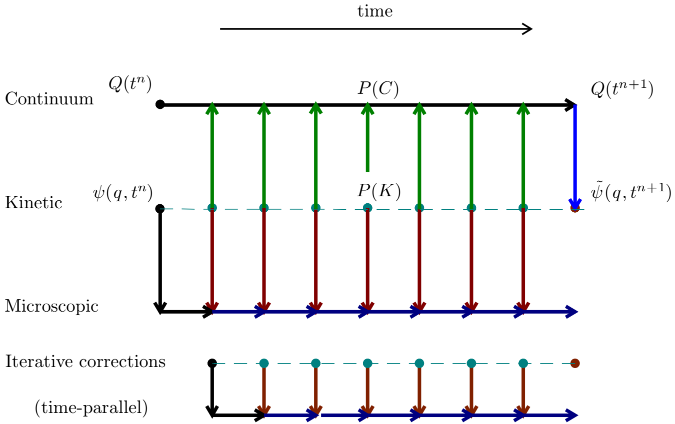
Microscopic verification of kinetic level

- Compare probability density estimates



Correct continuum evolution

- Runge-Kutta multistage update of continuum closure



tP-CKM

Continuum predictor imposes boundary condition constraints

- Microstate specified by $q \in \mathfrak{P} \subseteq \mathbb{R}^m$ within phase space $\mathfrak{P}$ of dimension $m \gg 1$
- Probability density $\psi(q,t)$, $P(q(t) \in \mathfrak{p}) = \int_{\mathfrak{p}} \psi(q,t)\,\mathrm{d}q$
- $G(q)$ microscopic generator of Q, $Q(t) = \int_{\mathfrak{P}} G(q)\,\psi(q,t)\,\mathrm{d}q$
- In particular, at end of continuum time step, $Q^{L+1} = \int_{\mathfrak{P}} G(q)\,\psi(q, T^{L+1})\,\mathrm{d}q$ are *constraints* on ψ
- Normalization constraint, $\int_{\mathfrak{P}} \psi(q, T^{L+1})\,\mathrm{d}q = 1$

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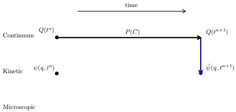
$C \to K$ Minimal entropy modification of ψ



- Modify ψ^n to incorporate new constraints at t^{n+1}

$$\int G_i(q)\psi^{n+1}(q)\mathrm{d}q = C_i, 1 \leq i \leq N$$

- Define relative entropy (Kullback-Leibler)

$$\mathcal{D}(\psi^{n+1}|\psi^n) = \int \psi^{n+1} \log\left(\frac{\psi^{n+1}}{\psi^n}\right) \mathrm{d}q$$

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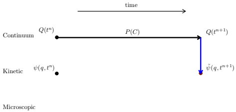

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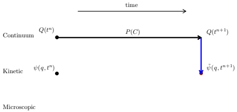

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- $\exists \psi^{n+1}$ that minimizes information distance
- Optimal ψ^{n+1} found by Lagrange multipliers

$$\inf_{\lambda_i} \sup_{\psi} \left[-\mathcal{D}(\psi|\psi^n) + \sum_{i=1}^{N} \lambda_i \left(\int G_i(q)\psi(q)\mathrm{d}q - C_i \right) \right]$$

- N-parameter family of candidate solutions

$$\psi_\lambda = \frac{1}{Z(\lambda)} \psi^n(q) \exp\left(\sum_{i=1}^{N} \lambda_i G_i(q) \right)$$

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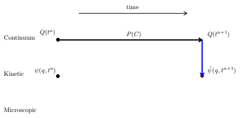
$C \to K$ FENE-P predictor



- Impose continuum constraints
  - Example: FENE-P predictor
  - Dumbbell model $q \equiv r$
  - Continuum prediction

$$\mathbf{T}^{n+1} = < r^{n+1} r^{n+1} >$$

$$\partial_t \mathbf{T} + v \cdot \nabla \mathbf{T} - \nabla v \mathbf{T} - \mathbf{T} (\nabla v)^T = \frac{4kT}{\zeta} I - \frac{4H/\zeta}{1 - tr(\mathbf{T})/q_0^2} \mathbf{T}$$

- $\int \mathbf{G}(r) \psi^{n+1}(r) \mathrm{d}r = \mathbf{T}^{n+1}$, $\mathbf{G}(r) = r\, r$

- Solve: $\frac{1}{Z(\lambda)} \frac{\partial Z(\lambda)}{\partial \lambda_i} = \mathbf{T}_i^{n+1}$
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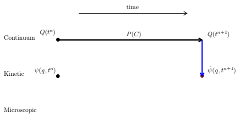

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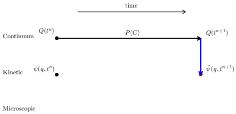

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Modification of dumbbell pdf under flow

- Initial PDF $\psi(\mathbf{r}, t^n) = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp\left[-\frac{(\mathbf{r}-\mathbf{r}_n)^2}{2\sigma_n^2}\right]$

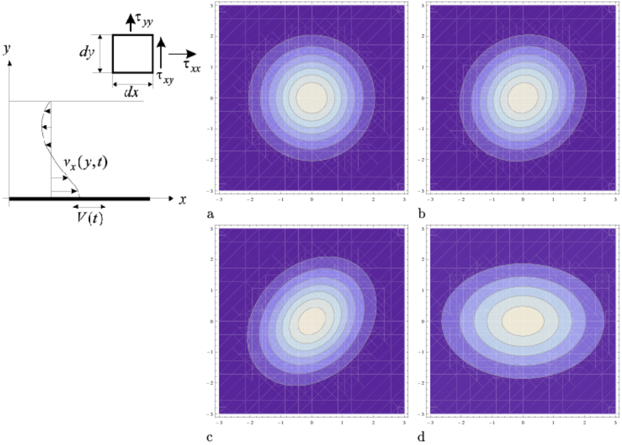

Figure 1. PDF $\psi(x,y)$: (a) no flow; (b) shear flow $T_{xy} = 0.1$; (c) shear flow $T_{xy} = 0.25$; (d) Dilatational flow $T_{xx} = 0.25$

Bregman divergence

- Definition: $\mathcal{D}(\psi, \varphi) = \int_{\mathfrak{P}} B(\psi(q), \varphi(q))\, \mathrm{d}q$

$$\delta\mathcal{H}\left(\psi, \psi^L, \lambda\right) = -\int_{\mathfrak{P}} \left[\frac{\partial B\left(\psi(q), \psi^L(q)\right)}{\partial \psi} - \sum_{i=0}^{M} \lambda_i G_i(q)\right] \delta\psi \mathrm{d}q$$

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- Generating function: $B_F(x, y) = F(x) - F(y) - (x - y) F'(y)$
- Euclidean distance: $B_E(x, y) = x^2 - y^2 - 2(x - y) \cdot y = (x - y)^2$
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  - a_j^L is mean of Gaussian distribution
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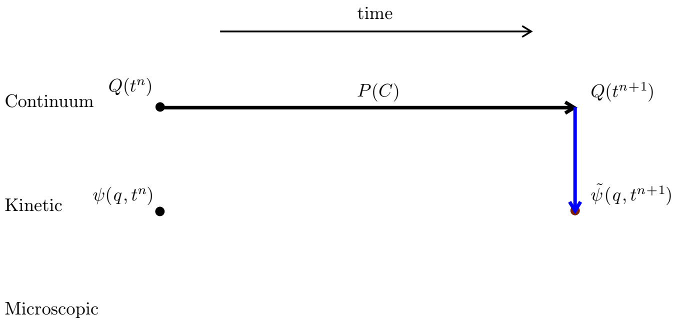
tP-CKM

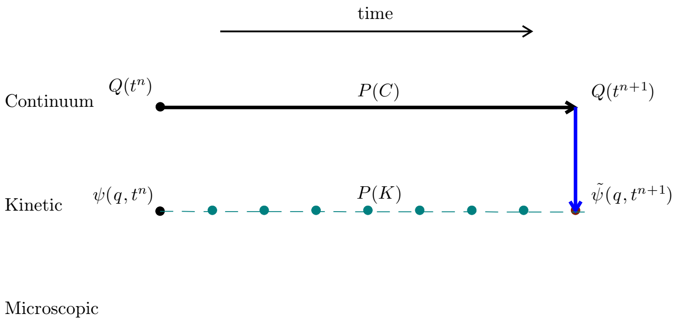
Impose continuum constraints on microconfiguration

- Modify previous probability density



Kinetic-level time evolution

- Generate intermediate probability densities



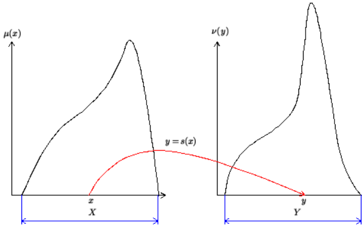
$K(t^n) \longleftrightarrow K(t^{n+1})$ Optimal transport of ψ

- Given two pdf's $\psi^0 : A \to \mathbb{R}$, $\tilde{\psi}^1 : B \to \mathbb{R}$
- Transferance plan $T : A \to B$

$$\int_{q \in P \subset A} \psi^0(q) \mathrm{d}q = \int_{q \in T(P) \subset B} \tilde{\psi}^1(q) \mathrm{d}q$$

- Optimal T minimizes Wasserstein distance

$$d_p(\psi^0, \tilde{\psi}^1) = \left(\inf_T \int |T(q) - q|^p \psi^0(q) \mathrm{d}q \right)^{1/p}$$



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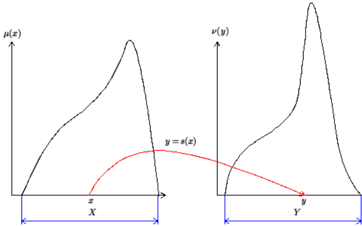

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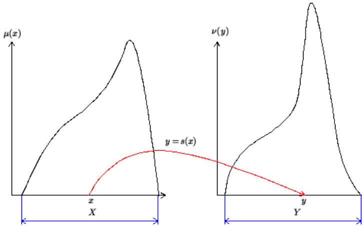

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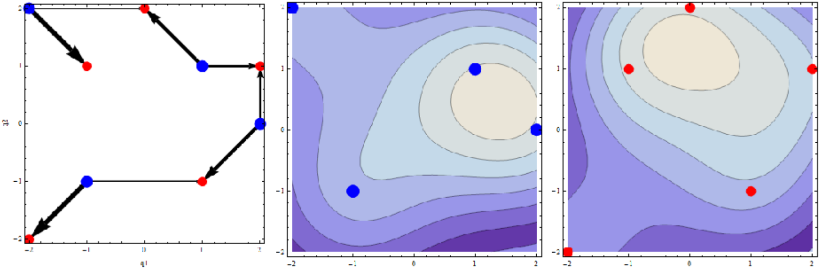
Example: discretely supported densities

- $\mu(x) = \sum_{i=1}^{m} \alpha_i \delta(x - x_i), \nu(y) = \sum_{j=1}^{n} \beta_j \delta(y - y_j)$



$K(t^n) \longleftrightarrow K(t^{n+1})$ Initial value problem for ψ

- Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} = \frac{\partial}{\partial q} \cdot \left(\frac{\partial \phi}{\partial q} \psi \right) + \frac{1}{\beta} \frac{\partial}{\partial q} \cdot \frac{\partial \psi}{\partial q}$$

- ϕ force potential
- Difficult to solve $q \in Q$, $\dim(Q) >> 1$
  - grid methods impractical
  - fast multipole methods work

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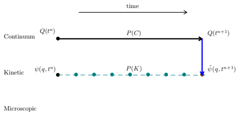

- Jordan, Kinderlehrer, Otto: $\psi(t)$ solves minimization problem

$$\min_{\psi}\left[\frac{1}{2}d_2(\psi^{(n-1)},\psi)+(\Delta t)F(\psi)\right]$$

- Steepest descent of free energy w.r.t. Wasserstein 2-distance

$$F(\psi)=E(\psi)+\frac{1}{\beta}S(\psi)$$

$$E(\psi)=\int\phi(q)\psi(q)\mathrm{d}q, S(\psi)=\int\psi(q)\log\psi(q)\mathrm{d}q$$

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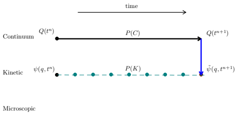

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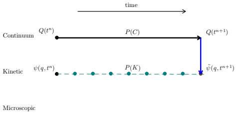
Interpolation of $\psi(q,t)$ time evolution

- JKL reformulation is just as hard as solving FP
- Interpolate between $\psi^n(q)$, $\tilde{\psi}^{n+1}(q)$
- Choose basis functions $B_l(q)$ (e.g. Gaussian kernels)
- Introduce approximation over $[t^n, t^{n+1}]$

$$\psi^{n,n+1}(t,q) = \sum_{l=1}^{L} c_l(t) B_l(q)$$



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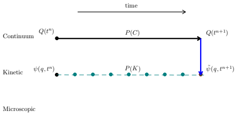

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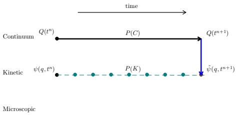

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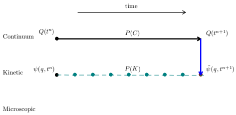

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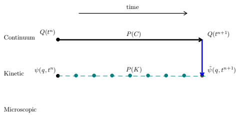
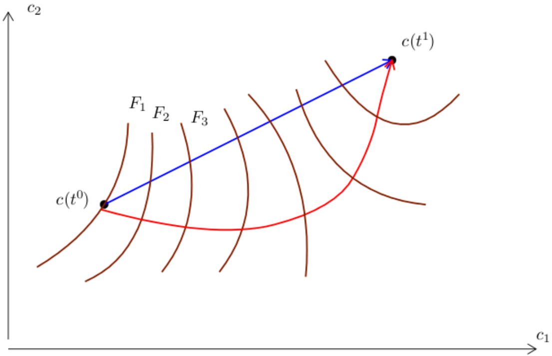
Gradient descent determines cubic interpolant

- Gradient in c-space, $\nabla_c F(\psi)$
- $F(\psi) = E(\psi) + S(\psi)/\beta$





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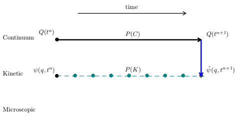

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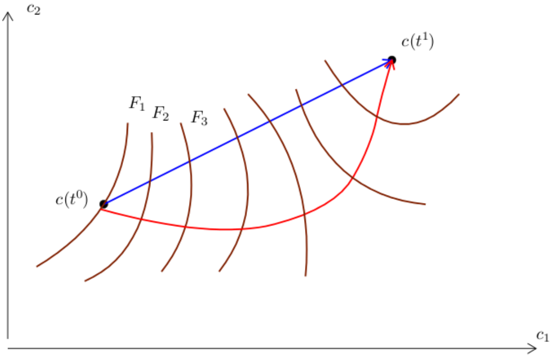

Radial Basis Function approximation

- Approximation over $[t^n, t^{n+1}]$

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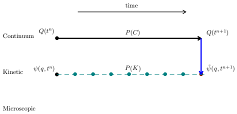
- Choose q_l in hypercylinder from $< q(t_1^n) >, < q(t_2^n) >, \ldots$
- Averages determined from microscopic-corrected PDF $P(K|M) \propto P(M|K)\, P(K)$ at each t^{n_j}



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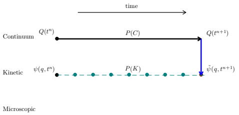

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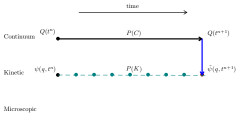

tP-CKM

1. Paradigm
2. Approach
3. C ↔ K
4. K ↔ M
5. Results
   - Time-parallel speedups
   - Scale communication
   - Complex viscoelastic flows

Compare DNS vs tPKM on viscoelastic shear flow

- Damped systems - few iterative refinement iterations
- Conservative systems - more iterative refinement iterations (SM, Proc. Comp. Sci. 1:745-752, 2010)

P	4	4	4	4	4	64	64	64	64	64
$\lg(H/\gamma)$	-2	-1	0	1	2	-2	-1	0	1	2
k	1	1	1	3	4	1	1	1	3	3
$\frac{\text{tPKM}}{\text{DNS}-\text{SDE}}$	**3.1**	**2.7**	**2.2**	**1.3**	**0.4**	**52**	**47**	**43**	**35**	**20**
% of possible	78	68	55	33	10	82	74	67	55	31

Table 1: Speedup (wall clock time) of tPKM algorithm by comparison to direct numerical simulation of the stochastic differential equations at the molecular scale.

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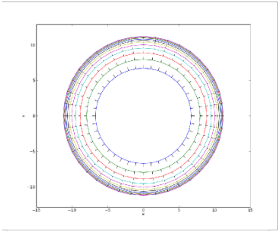
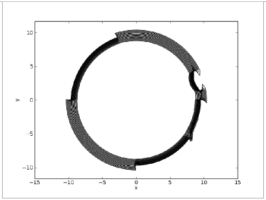
Application to cytoskeleton

- Apply interior pressure to circular cell membrane
- Test that micromechanics maintains symmetry (10^7 actin segments)
- Modify cytoskeleton-membrane attachment probability
- Observe bleb formation





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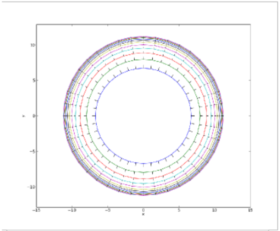

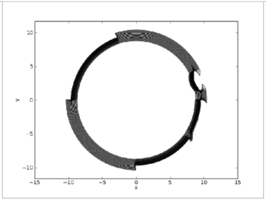

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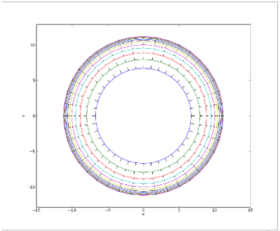

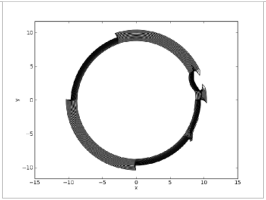

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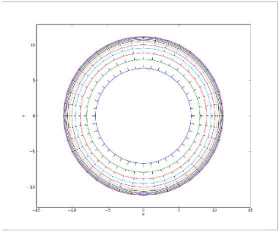
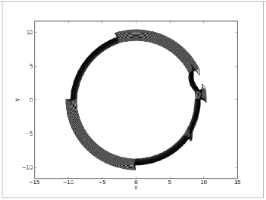
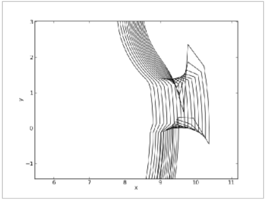
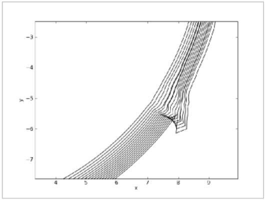




Bleb inflation, retraction

- Time sequence of membrane shapes
- Bleb inflation
- Bleb retraction
- (SM, J. Young, Springer Volume on Mechanobiology, 2010)





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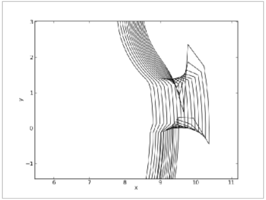

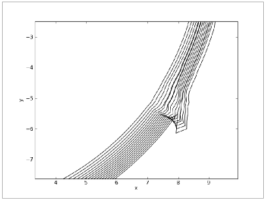

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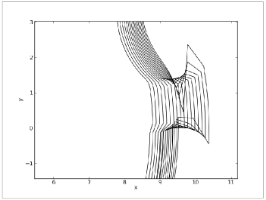

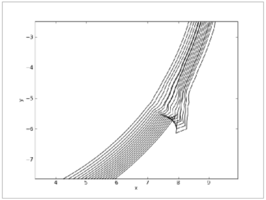

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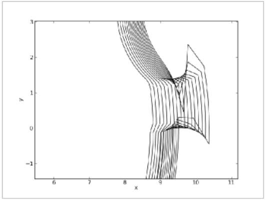
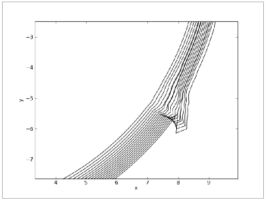
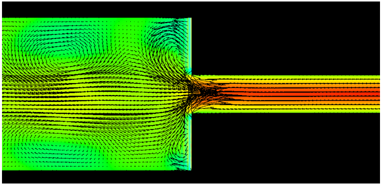




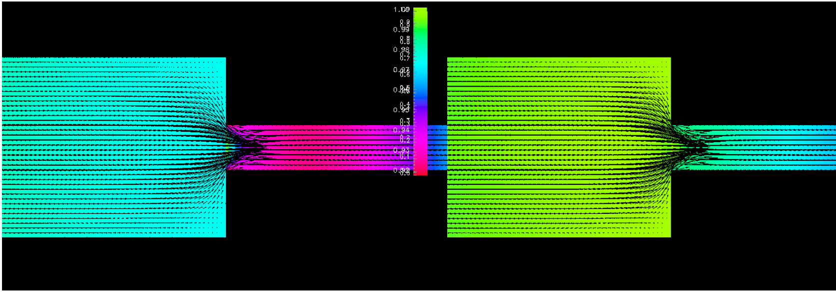
Viscoelastic contraction flow

- High Weissenberg number $We = 15$



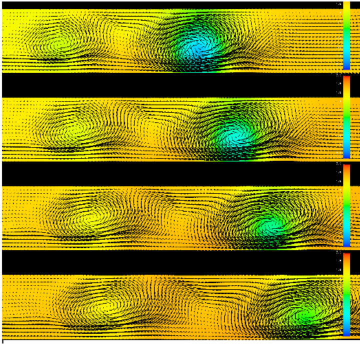
Model validity maps

- Compare Oldroyd-B vs FENE-P



Multiphysics

- Relevant to modeling coughing
- Viscoelastic fluid in contact with Newtonian fluid
- Entrainment of viscoelastic fluid by Newtonian fluid flow
- No phase interface imposed at continuum
- Phases distinguished by different microscopic forces



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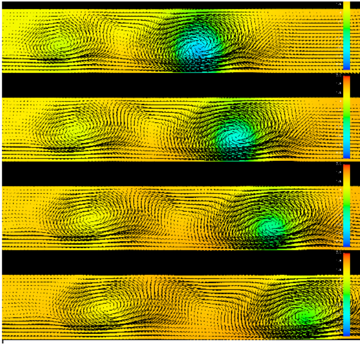

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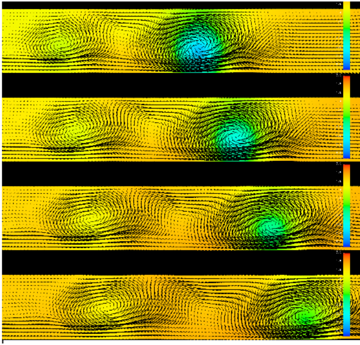

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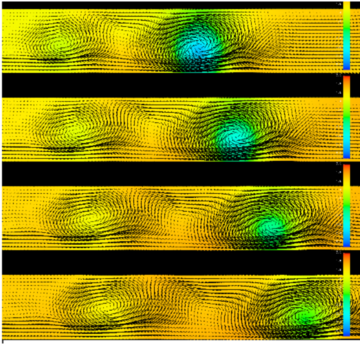

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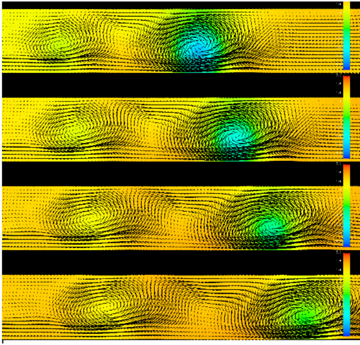
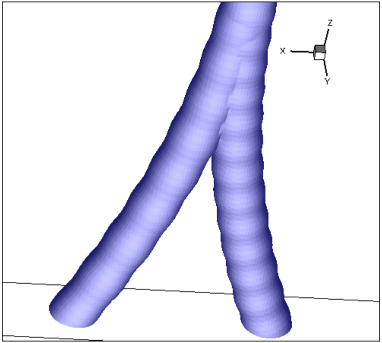


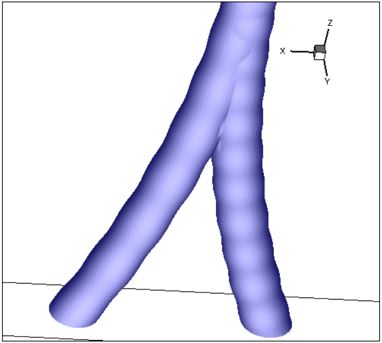
AirwayFewLinks

- Transient link gel model, small link lifetime
- Lattice Boltzmann core airflow
- Airway surface liquid entrainment



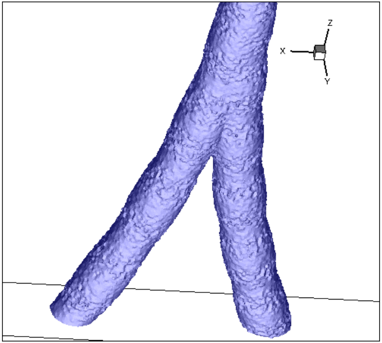
AirwayManyLinks

- Transient link gel model, long link lifetime
- Lattice Boltzmann core airflow
- Airway surface liquid entrainment



AirwayHighSpeed

- Transient link gel model, long link lifetime
- High-speed core airflow
- Lattice Boltzmann core airflow
- Airway surface liquid entrainment



tP-CKM conclusions

- Specifically designed for *non-equilibrated* phenomena
- Designed to expose problem parallelism to enable efficient computation (GPUs, many cores)
- Kinetic level as bridge between scales
- Approximate kinetic evolution through variational formulation
- Continuum predictor of kinetic PDF
- Kinetic predictor of microscopic evolution
- Kinetic compression of microscopic data (CPU ↔ GPU)
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- Gregory Herschlag: polymer microstructure formation during spin-casting (NSF-SOLAR, 2013 PhD)
- Dan Fovargue: lithotripsy fracture models (NIH, 2013 PhD)
- Anil Shenoy: anomalous diffusion in biomaterials, learning algorithms (NIH, 2014 PhD)
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