Weierstrass Institute for
Applied Analysis and Stochastics

Leibniz Association

Convergence of Coagulation–Advection Simulations

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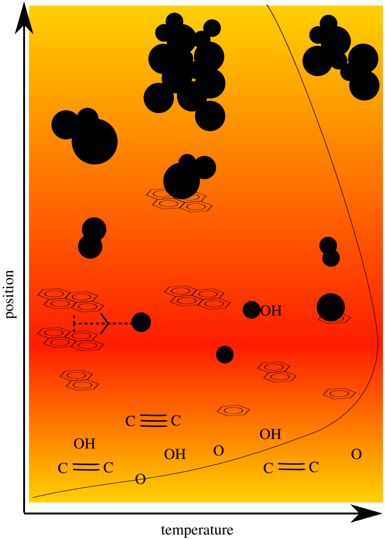
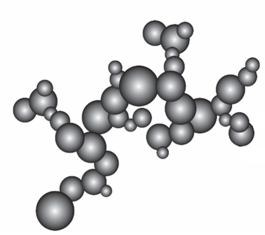
joint work with Wolfgang Wagner, Berlin

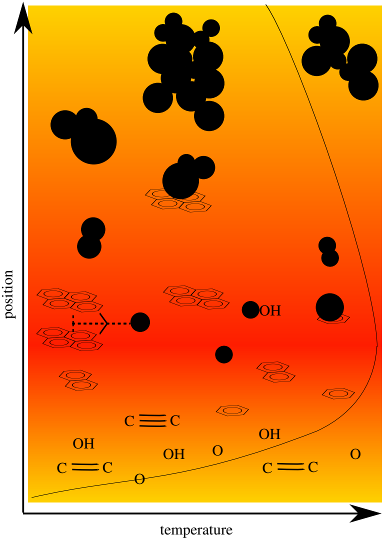
- Bounded region $\mathcal{X} = [0, L)$ of reacting laminar flow.
- Particle type space $\mathcal{Y}$.
- Particles incepted with intensity $I \geq 0$.
- Particles undergo surface growth at rate $\beta \geq 0$.
- Pairs of particles collide and coagulate according to $K \geq 0$, which models effects of diffusion.
- Particles drift at velocity $u > 0$.
- Particles simply flow out of the domain from its end.



$$
\begin{aligned}
\frac{\partial}{\partial t}c(t,x,y) + \nabla_x\left(u(x)c(t,x,y)\right)& \\
= I(x,y) + c(t,x,y-\delta)\beta\left(x,y-\delta\right) - c(t,x,y)\beta\left(x,y\right)& \\
+ \frac{1}{2}\iint_{\substack{y_1,y_2\in\mathcal{Y}:\\ y_1+y_2=y}} \mathrm{K}\left(x,y_1,x,y_2\right)c(t,x,y_1)c(t,x,y_2)\mathrm{d}y_1\mathrm{d}y_2& \\
- c(t,x,y)\int_{y_1\in\mathcal{Y}} \mathrm{K}\left(x,y,x,y_1\right)c(t,x,y_1)\mathrm{d}y_1&
\end{aligned}
$$



- Boundary and initial conditions.
- Homogeneous form: M. von Smoluchowski, “Drei Vorträge über Diffusion, Brownsche Molekularbewegung und Koagulation von Kolloidteilchen”, *Physik. Zeitschr.*, XVII:585–599,(1916).



- Complex particles mean high dimensional phase space.
- Coagulation has terms like

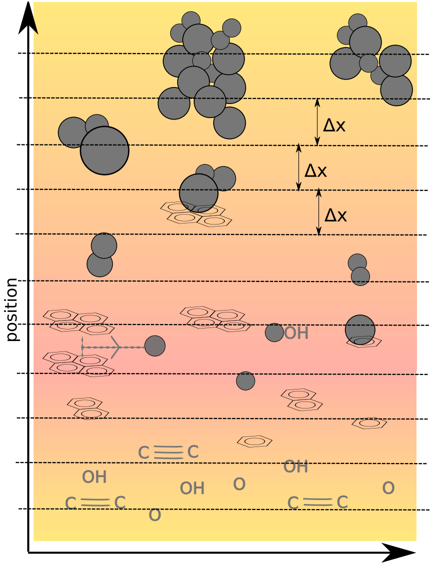
$$c(t,x,y)\int_{y_1\in\mathcal{Y}} \mathrm{K}(x,y,x,y_1)\, c(t,x,y_1)\mathrm{d}y_1.$$

- Moment closures are messy and approximate.
- Complexity is exponential in phase space discretisation length.
- Use Monte Carlo.

Weak formulation is natural for particle systems viewed through their empirical measures:

$$
\begin{aligned}
&\frac{\partial}{\partial t}\int_{\mathcal{X}\times\mathcal{Y}}\phi(x,y)c(t,x,y)\mathrm{d}x\mathrm{d}y \\
&\qquad\qquad +\int_{\mathcal{X}\times\mathcal{Y}}\phi(x,y)\nabla_x\left(u(x)c(t,x,y)\right)\mathrm{d}x\mathrm{d}y \\
&=\int_{\mathcal{X}\times\mathcal{Y}}\phi(x,y)I(x,y)\mathrm{d}x\mathrm{d}y \\
&\qquad +\int_{\mathcal{X}\times\mathcal{Y}}\left[\phi(x,y+\delta)-\phi(x,y)\right]\beta\left(x,y\right)c(t,x,y)\mathrm{d}x\mathrm{d}y \\
&\qquad +\frac{1}{2}\int_{\mathcal{X}}\int_{\mathcal{Y}\times\mathcal{Y}}\left[\phi(x,y_1+y_2)-\phi(x,y_1)-\phi(x,y_2)\right] \\
&\qquad\qquad\qquad c(t,x,y_1)c(t,x,y_2)\mathrm{K}\left(x,y_1,x,y_2\right)\mathrm{d}y_1\mathrm{d}y_2\mathrm{d}x.
\end{aligned}
$$

- Investigate methods that approximate the PBE.
- Grid spacing Δx, $\mathcal{X} = \bigcup_{j=1}^{J} \mathcal{X}_j$.
- Simplified models of the physical particle system are good sources of ideas for numerical methods.
- Overall goal is understanding the convergence of the empirical measures.
- This work focuses on exit boundaries.
- Diffusion in coagulation kernel—model for smallest scale.
- For numerical purposes split transport and reaction terms.



- Infinite homogeneous box, no flow:
  - Boltzmann setting: Wagner 92
  - Coagulation: Jeon 98, Norris 99
  - Famous review by Aldous 99
  - More general interactions: Eibeck & Wagner 03, Kolokoltsov book 10
- Diffusion in infinite domain: via jump process Guiaş 01
- Diffusion in infinite domain: via SDE Deaconu & Fournier 02
- Hammond, Rezakhanlou & co-workers 06-10
- Relative compactness in law for advection in 1-d finite domain: P. 13
- Gas dynamics.

- Need a sequence of Markov Chains to study convergence; index n.
- Replace continuum with finite, computable number of particles.
- Scaling factor n: Inverse of concentration represented by one computational particle.
- Coagulation y_1 and y_2 at rate $K(y_1, y_2)/2n\Delta x$ (ignore x dependence).
- Other delocalisation methods possible.
- Formation of new particles at rate $\Delta x n I$ throughout the cell.
- Velocity $u > 0$ bounded away from 0, u' bounded, streaming step split.
- Particles absorbed at end of reactor.

- Individual particle and position an element of $\mathcal{X}' = \mathcal{X} \times \mathcal{Y}$.
- Fock state space for the particle systems $E = \bigcup_{k=0}^{\infty} \mathcal{X}'^k$.
- Let $\psi : \mathcal{X}' \to \mathbb{R}$ and define $\psi^{\oplus} : E \to \mathbb{R}$ by $\psi^{\oplus}(x_1, \ldots x_k) = \sum_{j=1}^{k} \psi(x_j)$.
- $X_n(t)$ is the E-valued process.
- $N(X_n(t))$ is the number of particles.
- $X_n(t, i) \in \mathcal{X}'$ is the location and type of the i-th particle.

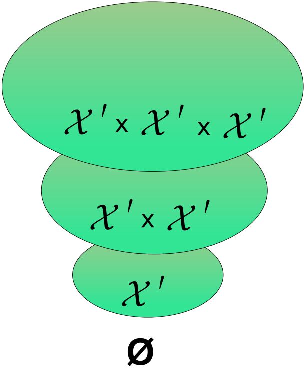


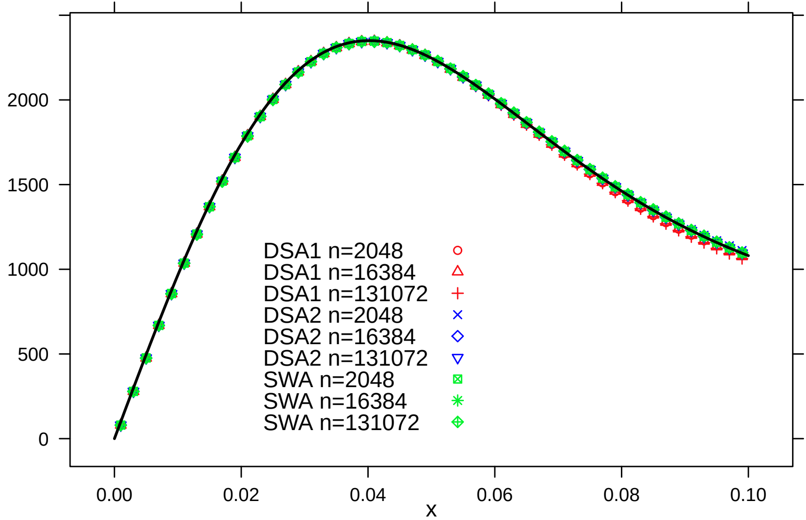
Figure: The disjoint union E.

Let $X \in E$, $X = (X(1), \dots, X(N(X)))$, then the generators A_n satisfy

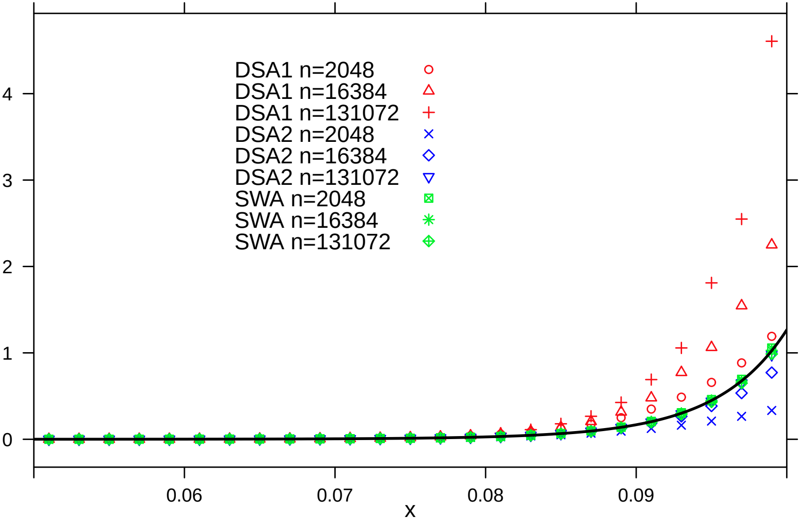
$$
\begin{aligned}
A_n \psi^{\oplus}(X) = A_n \left(\sum_{i=1}^{N(X)} \psi(X(i)) \right) \\
= n \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y) I(\mathrm{d}x, \mathrm{d}y) + (u \nabla \psi)^{\oplus}(X) + \\
\frac{1}{2} \sum_{j=1}^{J} \sum_{\substack{i_1, i_2 = 1 \\ i_1 \neq i_2}}^{N(X)} \left[\psi\big(X(i_1) + X(i_2)\big) - \psi(X(i_1)) - \psi(X(i_2)) \right] \\
\frac{K(X(i_1), X(i_2))}{n \Delta x} \mathbb{1}_{\mathcal{X}_j}(X(i_1)) \mathbb{1}_{\mathcal{X}_j}(X(i_2)).
\end{aligned}
$$

- Poissonian inception with rate I,
- advection with velocity u,
- coagulations of $X(i_1)$ and $X(i_2)$ at rate $K(X(i_1), X(i_2)) / 2n\Delta x$,
- exits at L require $\psi = 0$ there.

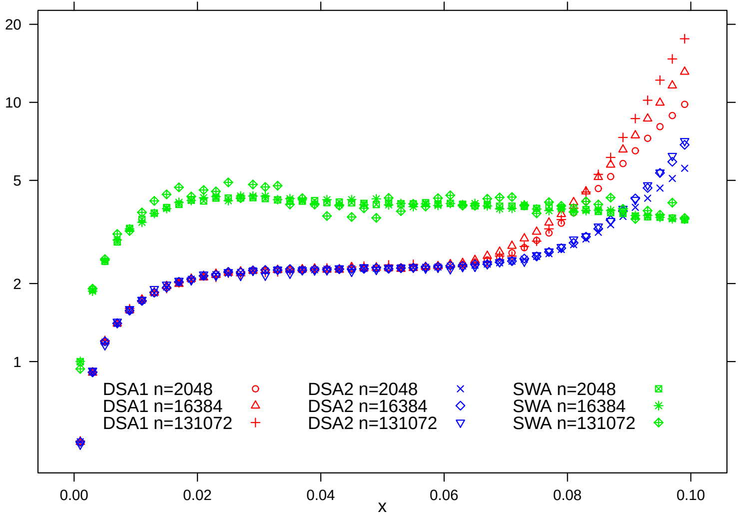
Simple problem, steady state concentration (zeroth moment) has closed form solution.



Second mass moment:



Standard deviation of concentration (zeroth mass moment) renormalised by mean and $\sqrt{n}$:



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&= n \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y) I(\mathrm{d}x, \mathrm{d}y) + (u \nabla \psi)^{\oplus}(X) + \\
&\frac{1}{2} \sum_{j=1}^{J} \sum_{\substack{i_1, i_2 = 1 \\ i_1 \neq i_2}}^{N(X)} \left[\psi\big(X(i_1) + X(i_2)\big) - \psi(X(i_1)) - \psi(X(i_2)) \right] \\
&\qquad \frac{K(X(i_1), X(i_2))}{n \Delta x} \mathbb{1}_{\mathcal{X}_j}(X(i_1)) \mathbb{1}_{\mathcal{X}_j}(X(i_2)).
\end{aligned}$$

- Poissonian inception with rate I,
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- exits at L require $\psi = 0$ there.

Definition

The empirical measure process, which is $\mathbb{D}(\mathbb{R}_0^+, \mathcal{M}(E))$ valued, is given by

$$\mu_t^n = \frac{1}{n} \sum_{i=1}^{N(X_n(t))} \delta_{X_n(t,i)} \,.$$

Thus

$$\psi^{\oplus}(X_n(t)) \equiv \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x, \mathrm{d}x).$$

and adapting the generator to measures find $\mathcal{A}$ a martingale characterization

$$\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x, \mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_0^n(\mathrm{d}x, \mathrm{d}y) \\ - \int_0^t \int_{\mathcal{X}\times\mathcal{Y}} \mathcal{A}(\mu_s^n)\psi(x,y)\mu_s^n(\mathrm{d}x, \mathrm{d}y)\mathrm{d}s = M_n^{\psi}(t) + \mathcal{O}(1/n).$$

Theorem (P. 13)

If inception I, velocity u, particle residence times, and coagulation kernel K are bounded, then the μ^n are weakly relatively compact in distribution so there is a limit with paths in $\mathbb{D}(\mathbb{R}_0^+, \mathcal{M}(E))$.

Proof.

By Jakubowski (1986) it is sufficient to check

- the corresponding result for the real valued processes $\int_{\mathcal{X}\times\mathcal{Y}} \psi(x, y)\mu_t^n(\mathrm{d}x, \mathrm{d}x)$,
- a tightness condition for the μ_t^n.

The tightness condition is established using the Poissonian nature of the inflow and the upper bound on the residence times. □

I think one also has exponential tightness.

Recall

$$\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x,\mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_0^n(\mathrm{d}x,\mathrm{d}y) - \int_0^t \int_{\mathcal{X}\times\mathcal{Y}} \mathcal{A}(\mu_s^n)\psi(x,y)\mu_s^n(\mathrm{d}x,\mathrm{d}y)\mathrm{d}s = M_n^\psi(t) + \mathcal{O}(1/n).$$

- $\mathbb{E}\left[\sup_{s\le t} M_n^\psi(t)^2\right] = \mathcal{O}(1/n)$ so passing to the limit

$$\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t(\mathrm{d}x,\mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_0(\mathrm{d}x,\mathrm{d}y) - \int_0^t \int_{\mathcal{X}\times\mathcal{Y}} \mathcal{A}(\mu_s)\psi(x,y)\mu_s(\mathrm{d}x,\mathrm{d}y)\mathrm{d}s = 0.$$

- Equation has a unique solution (Banach ODE analysis).
- Processes converge to this unique solution with probability 1.

Recall the noise Martingale

$$M_n^\psi(t) := \frac{1}{n}\psi^\oplus\left(X_n(t)\right) - \frac{1}{n}\int_0^t A_n\psi^\oplus\left(X_n(s)\right)\mathrm{d}s$$

these can be decomposed as

$$M_n^\psi(t) = \sum_{k=1}^{T_n(t)} \xi_{n,k} + \mathcal{O}(1/n).$$

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Already noted

$$\mathbb{E}\left[\sup_{s\leq t} M_n^\psi(s)^2\right] \sim \mathcal{O}(1/n),$$

but by working a little harder

$$n\mathbb{E}\left[M_n^\psi(t)^2\right] = \mathbb{E}\left[\sum_{k=1}^{T_n(t)}\left(\sqrt{n}\xi_{n,k}\right)^2\right] + \mathcal{O}(1/\sqrt{n}) \to \int_0^t \sigma(s)^2\mathrm{d}s.$$

(Note: σ is explicit and deterministic.)

- $\sqrt{n}M_n^{\psi}(t) \to B_{v(t)}$ so, informally

$$\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x,\mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_0^n(\mathrm{d}x,\mathrm{d}y)$$

$$- \int_0^t \int_{\mathcal{X}\times\mathcal{Y}} \mathcal{A}(\mu_s^n)\psi(x,y)\mu_s^n(\mathrm{d}x,\mathrm{d}y)\mathrm{d}s \approx \sqrt{\frac{1}{n}}B_{v(t)}.$$

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- Even for large t, mistake to assume

$$\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x,\mathrm{d}y) \approx \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t(\mathrm{d}x,\mathrm{d}y) + \sqrt{\frac{1}{n}} B_{v(t)}.$$

- Concentrate on large times (after burn–in) so $v(t) \propto \sigma^2 t$.
- Useful simulation algorithms must drift towards true solution.
- Note that

$$\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x,\mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t(\mathrm{d}x,\mathrm{d}y)$$
$$\approx \int_0^t \left(\int_{\mathcal{X}\times\mathcal{Y}} \mathcal{A}(\mu_s^n)\psi(x,y)\mu_s^n(\mathrm{d}x,\mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \mathcal{A}(\mu_s)\psi(x,y)\mu_s(\mathrm{d}x,\mathrm{d}y) \right) \mathrm{d}s + \sqrt{\frac{1}{n}} B_{v(t)}.$$

- Ornstein–Uhlenbeck is a plausible model for

$$Y_t = \sqrt{n} \left(\int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_t^n(\mathrm{d}x,\mathrm{d}y) - \int_{\mathcal{X}\times\mathcal{Y}} \psi(x,y)\mu_0^n(\mathrm{d}x,\mathrm{d}y) \right),$$

which means

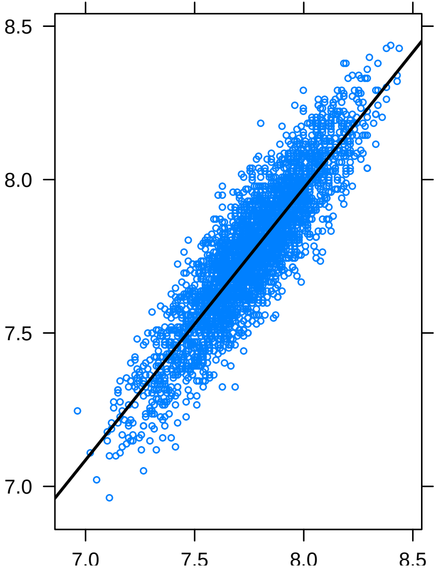
$$\mathrm{d}Y_t = \theta\left(m - Y_t\right)\mathrm{d}t + \sigma \mathrm{d}W_t.$$

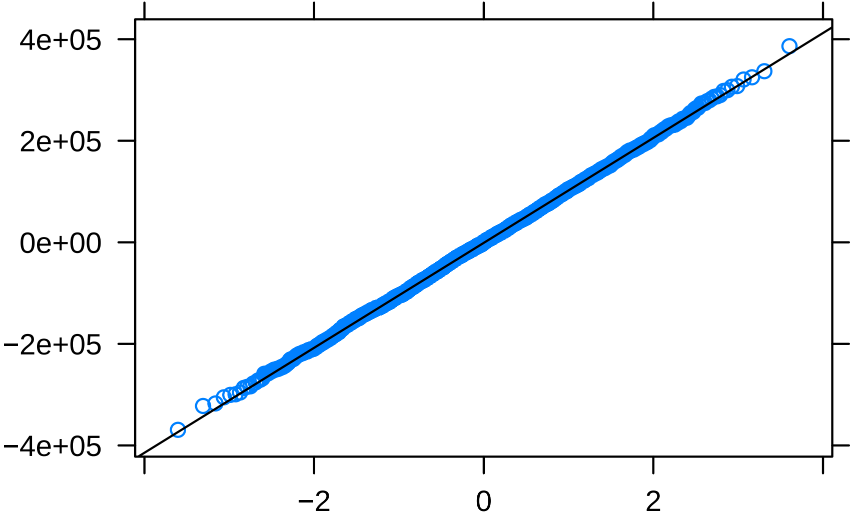
- Suppose Y is O-U, then

$$Y_{t_{i+1}} = Y_{t_i} e^{-\theta\Delta t} + m\left(1 - e^{-\theta\Delta t}\right) + \sigma\sqrt{\frac{1 - e^{-2\theta\Delta t}}{2\theta}} Z_i$$

where Z_i are iid $N(0,1)$.

- Observe a functional at t_i with spacing Δt, call the observations Y_{t_i}
- As a concrete example: Number of particles in $[0.175, 0.2]$:
- $e^{-\theta\Delta t} = 0.866 \pm 0.008$
- $m = 7.76 \pm 0.56$
- Mean reversion rate seems to depend on functional.
- How good is the assumption of normally distributed noise?





Straight line shows normal distribution matching 1st and 3rd quartiles of data.

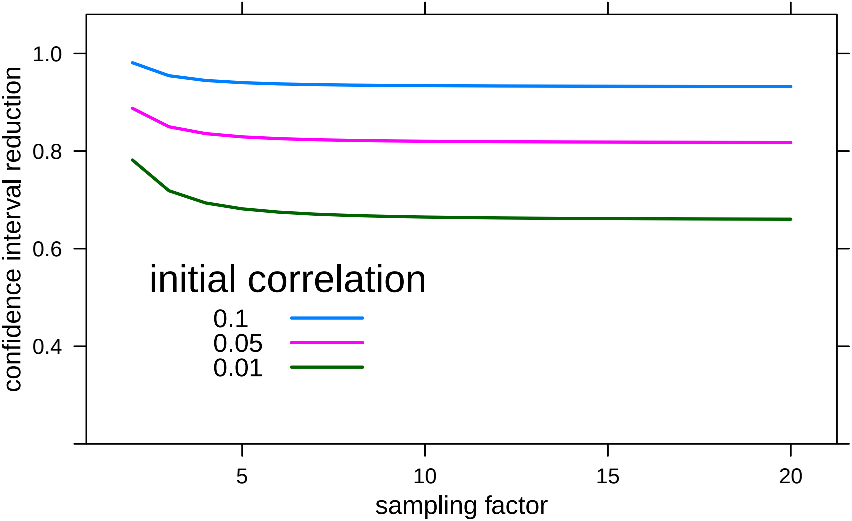
- Recall samples Y_i at times t_i, $i = 1, \ldots, i_{samp}$ with spacing Δt.
- Estimate mean as

$$\frac{1}{n} \sum_{i=1}^{i_{samp}} Y_i.$$

- Simulation cost is “burn-in” + $i_{samp} \Delta t$.
- Variance of estimator is

$$\mathrm{var}\left(\frac{1}{i_{samp}} \sum_{i=1}^{i_{samp}} Y_i \right) = \frac{\sigma^2}{2 i_{samp} \theta} \left(1 + \frac{2e^{-\theta \Delta t}}{1 - e^{-\theta \Delta t}} \right) + \mathcal{O}\left(\frac{1}{i_{samp}^2} \right).$$

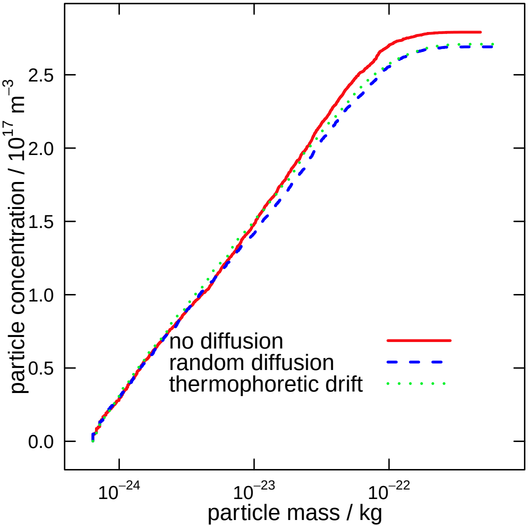
- For fixed cost, variance is monotone decreasing in $i_{samp} \propto 1/\Delta t$.
- Practical considerations will intervene before i_{samp} gets too big / Δt too small.



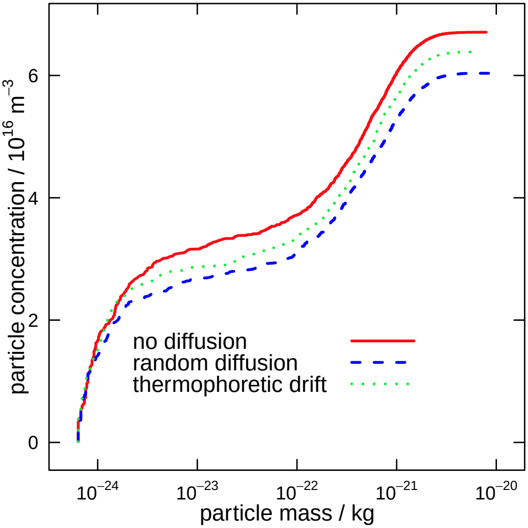
confidence interval reduction
1.0
0.8
0.6
0.4
5
10
15
20
sampling factor
initial correlation
0.1
0.05
0.01

A Sooting Flame with Thermophoresis

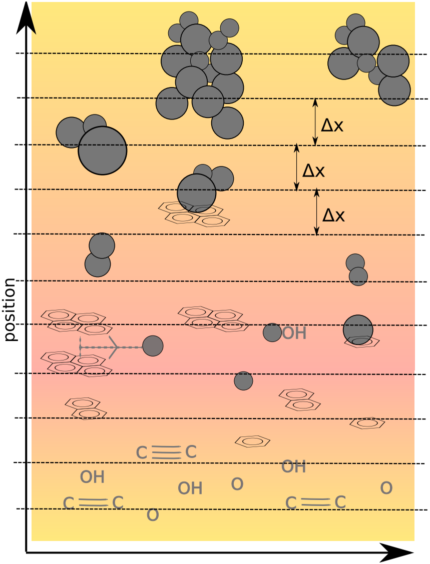
- Appel-Bockhorn-Frenklach soot model with spherical particles.
- Different transport models (increasing complexity)
  - advection,
  - advection with thermophoresis adjustment,
  - advection and diffusion.
- Uniform spatial grid (!) Δx.
- Splitting time Δt.
- Max particles per cell n.
- Pre-calculated chemical conditions (including u) taken from an old study courtesy of Jasdeep Singh.
- Weighted particles for performance reasons.



- Particle distribution around $x = 2.0625 \times 10^{-3}$.
- Difference in M_0 peaks shown here.
- M_0 is the right hand end point of the curves.



- Particle distribution around $x = 6.0625 \times 10^{-3}$.
- Note change of scales from previous figure.
- Not yet able to assess statistical significance.



- Ornstein–Uhlenbeck model for fluctuations useful.
- Decorrelation times can be estimated.
- Limited advantage when sampling already near optimal.
- Results from a wider range of sampling parameters can be interpreted.
- Open questions: Gradient flow, spectral gap, log Sobolev inequality.