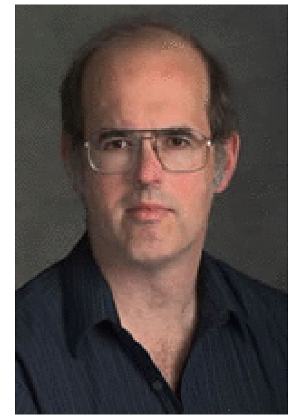
Fluctuating Hydrodynamics and Direct Simulation Monte Carlo



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Regimes for Dilute Gases

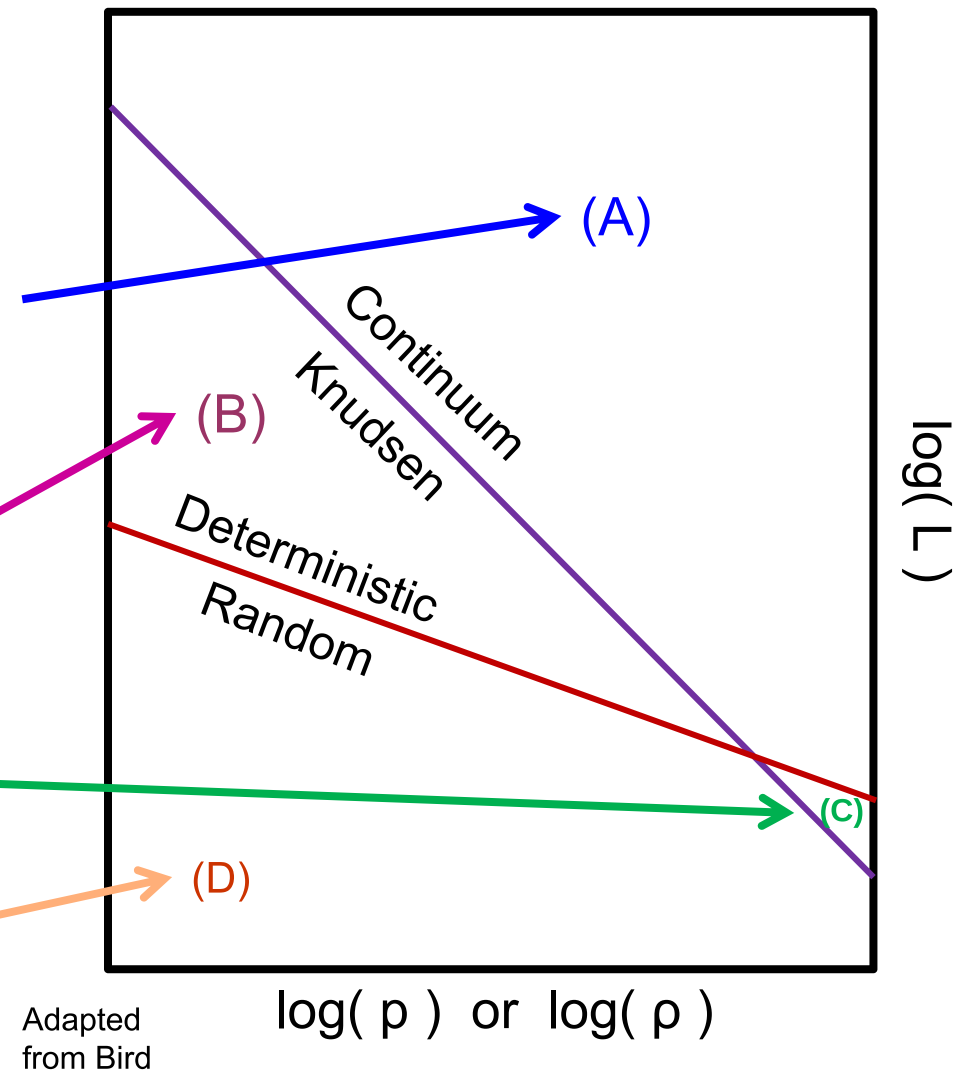
Continuum vs. Knudsen
Deterministic vs. Random

(A) Continuum, Deterministic:
Fluid mechanics & CFD

(B) Knudsen, Deterministic:
Kinetic theory & RGD

(C) Continuum, Random:
Fluctuating hydrodynamics

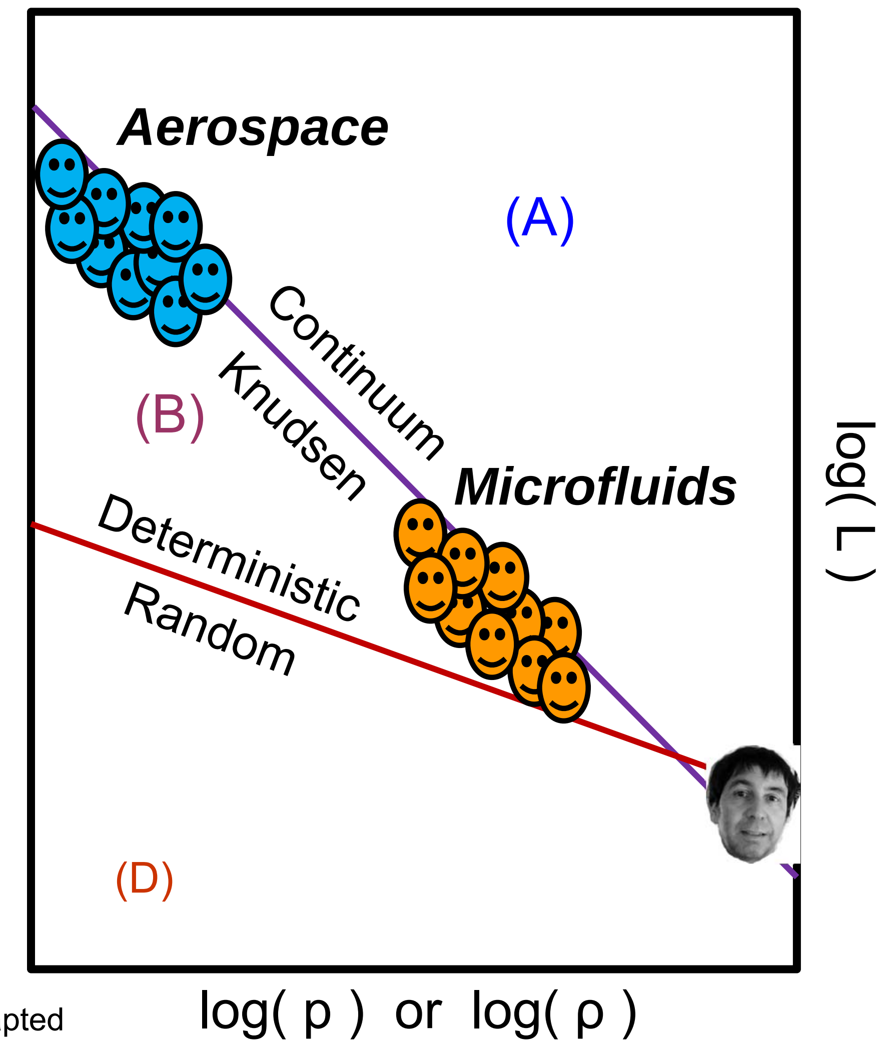
(D) Knudsen, Random



DSMC Simulations

DSMC can be used for *all* regimes but is primarily used in the Knudsen regime due to computational efficiency.

DSMC also useful for the study of fluctuations.

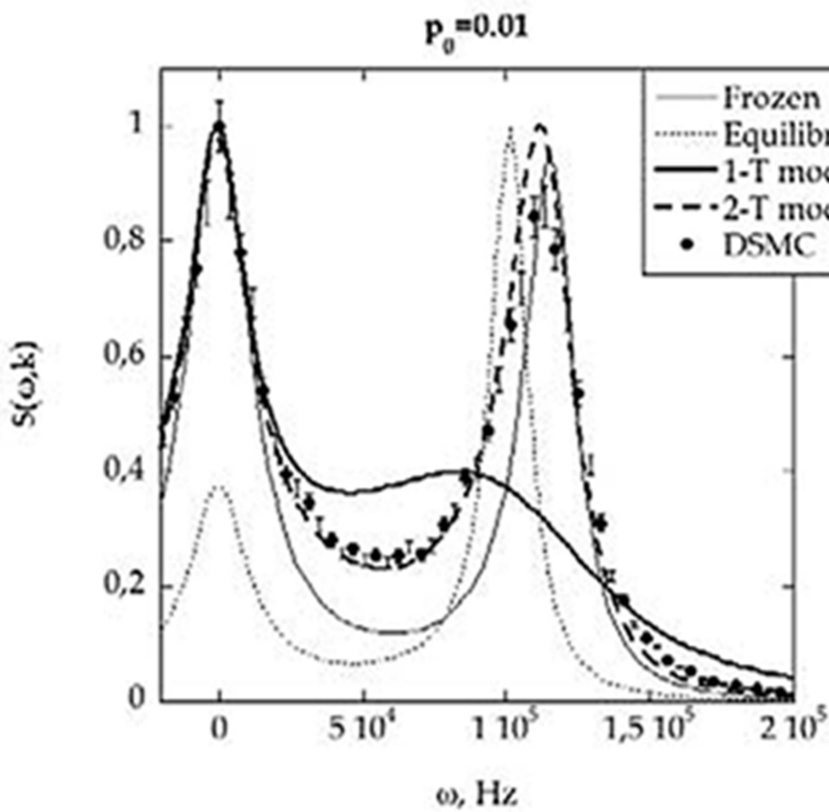


Adapted from Bird

Fluctuations in DSMC

Fluctuations in DSMC are <u>not</u> due to Monte Carlo; they are physically correct at hydrodynamic and kinetic scales.

Fluctuation spectra at equilibrium may be used to measure transport properties (e.g., contribution of internal energy to bulk viscosity).



D. Bruno, 27th RGD Proceedings (2011)

Fluctuations & Statistical Error

Fractional error in fluid velocity

$$E_{velocity} \approx \frac{1}{\sqrt{SN}} \frac{1}{\mathrm{Ma}}$$

where S is number of samples, Ma is Mach number.

For desired accuracy of $E_{velocity}$ = 1%, N = 100 particles/cell

$$S \approx \frac{1}{N\mathrm{Ma}^2 E_{velocity}^2} \propto \frac{1}{\mathrm{Ma}^2}$$

$S \approx 10^2$ samples for Ma =1.0 (Aerospace flow)
$S \approx 10^8$ samples for Ma = 0.001 (Microscale flow)

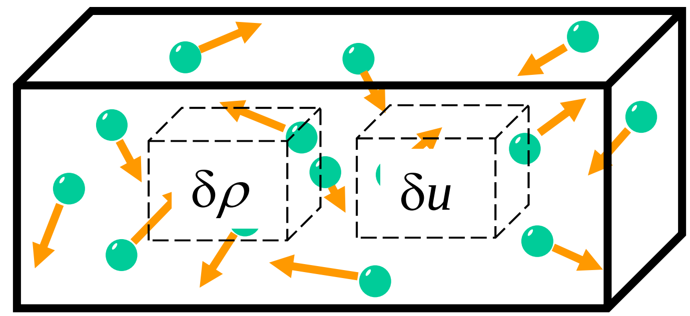
N. Hadjiconstantinou, ALG, M. Bazant, and G. He, *J. Comp. Phys.* **187** 274-297 (2003).

Correlations of Fluctuations

At equilibrium, fluctuations of conjugate hydrodynamic quantities are uncorrelated. For example, density is uncorrelated with fluid velocity and temperature,

$$\langle \delta\rho(x,t)\delta u(x',t) \rangle = 0$$

$$\langle \delta\rho(x,t)\delta T(x',t) \rangle = 0$$



Out of equilibrium, (e.g., gradient of temperature or shear velocity) correlations appear.

Fluctuating Navier-Stokes PDEs

Landau introduced fluctuations into the Navier-Stokes equations by adding white noise fluxes of stress and heat.

$$\partial \mathbf{U}/\partial t + \nabla \cdot \mathbf{F} = \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{S} \quad \text{where} \quad \mathbf{U} = \begin{pmatrix} \rho \\ \mathbf{J} \\ E \end{pmatrix} \begin{array}{l} \text{Mass} \\ \text{Momentum} \\ \text{Energy} \end{array}$$

Hyperbolic Fluxes | Parabolic Fluxes | Stochastic Fluxes

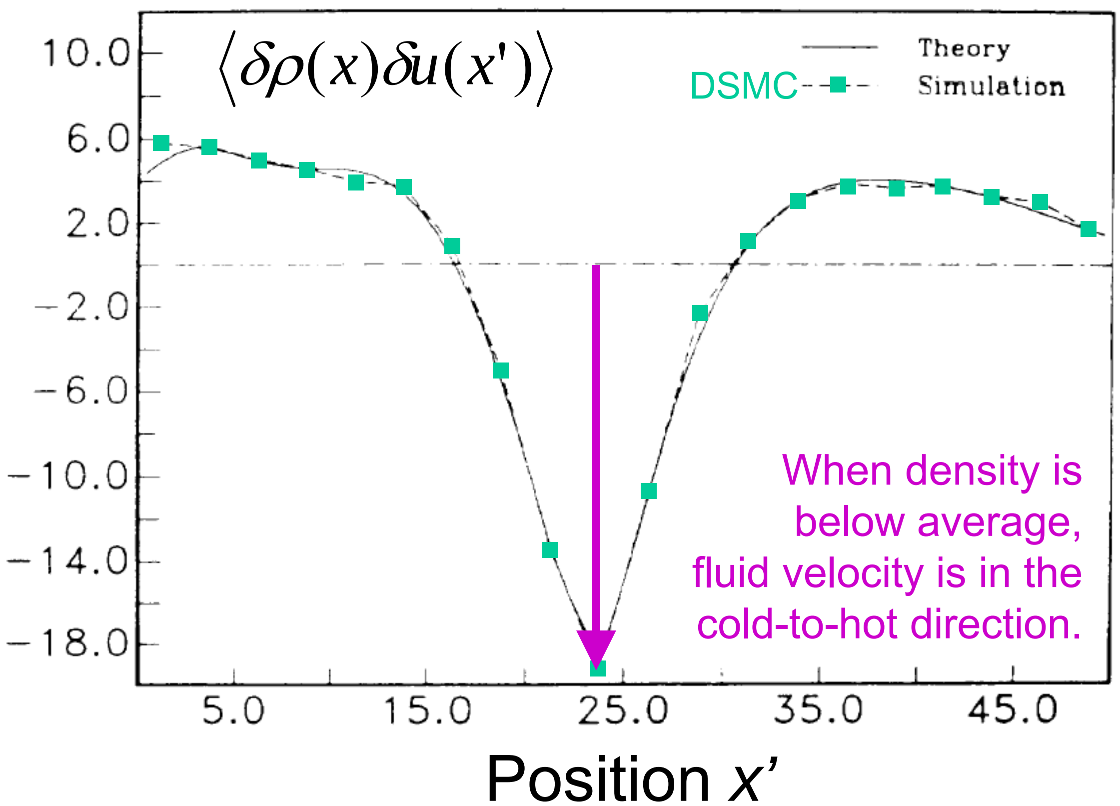
$$\mathbf{F} = \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v}\mathbf{v} + P\mathbf{I} \\ (E+P)\mathbf{v} \end{pmatrix} \; \mathbf{D} = \begin{pmatrix} 0 \\ \tau \\ \kappa \nabla T + \tau \cdot \mathbf{v} \end{pmatrix} \; \mathbf{S} = \begin{pmatrix} 0 \\ \mathcal{S} \\ \mathcal{Q} + \mathbf{v} \cdot \mathcal{S} \end{pmatrix},$$

$$\langle \mathcal{S}_{ij}(\mathbf{r},t)\mathcal{S}_{k\ell}(\mathbf{r}',t')\rangle = 2k_B\eta T \left(\delta^K_{ik}\delta^K_{j\ell} + \delta^K_{i\ell}\delta^K_{jk} - \tfrac{2}{3}\delta^K_{ij}\delta^K_{k\ell}\right)\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

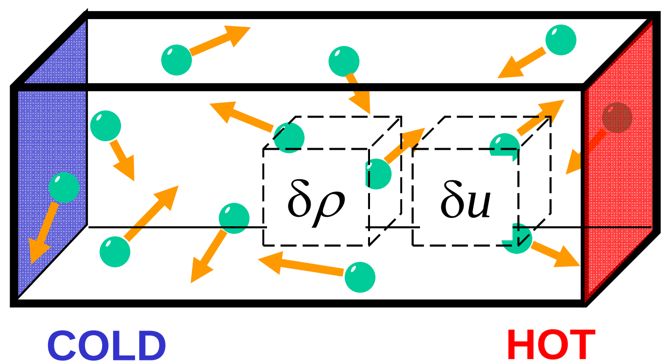
$$\langle \mathcal{Q}_i(\mathbf{r},t)\mathcal{Q}_j(\mathbf{r}',t')\rangle = 2k_B\kappa T^2\delta^K_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

Density-Velocity Correlation

Correlation of density-velocity fluctuations under ∇T



Theory is Landau-Lifshitz fluctuating hydrodynamics



ALG, *Phys. Rev. A* **34** 1454 (1986).
(My first DSMC paper)

Fluctuation Examples

Show three examples in which non-equilibrium fluctuations produce interesting physical or numerical effects:

- Anomalous fluid velocity and temperature in DSMC
- Enhancement of diffusion by fluctuations
- Fluctuations in reaction – diffusion problems

In all cases Landau-Lifshitz fluctuating hydrodynamics serves as both a theoretical approach and the basis for numerical simulations, complementing DSMC.

Fluctuation Examples (1)

- Anomalous fluid velocity and temperature in DSMC
- Enhancement of diffusion by fluctuations
- Fluctuations in reaction – diffusion problems

Due to non-equilibrium correlations of fluctuations the measurement of instantaneous fluid velocity and instantaneous temperature in DSMC produces anomalous, un-physical results.

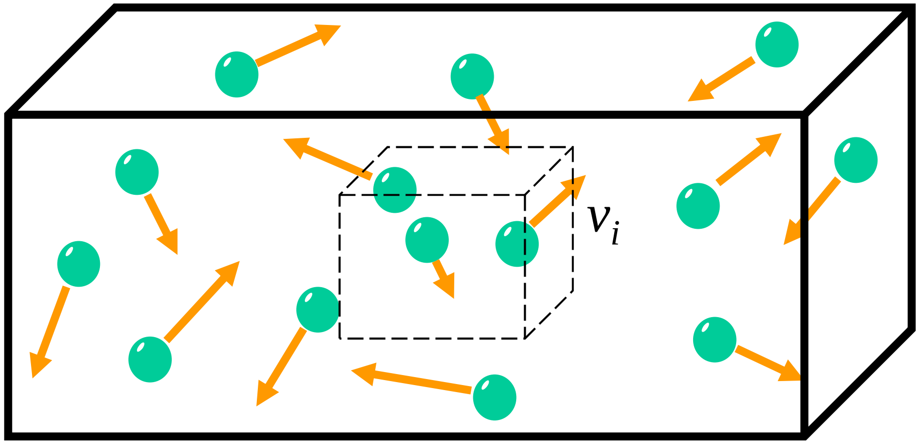
Instantaneous Fluid Velocity

Center-of-mass velocity in a cell C

$$u = \frac{J}{M} = \frac{\sum_{i \in C}^{N} m v_i}{mN}$$

Average particle velocity

$$\bar{v} = \frac{1}{N} \sum_{i \in C}^{N} v_i$$



Note that $u = \bar{v}$

Estimating Mean Fluid Velocity

Mean of instantaneous fluid velocity

$$\langle u \rangle = \frac{1}{S}\sum_{j=1}^{S} u(t_j) = \frac{1}{S}\sum_{j=1}^{S}\left(\frac{1}{N(t_j)}\sum_{i\in C}^{N(t_j)} v_i(t_j)\right)$$

where S is number of samples

Alternative estimate is the cumulative average

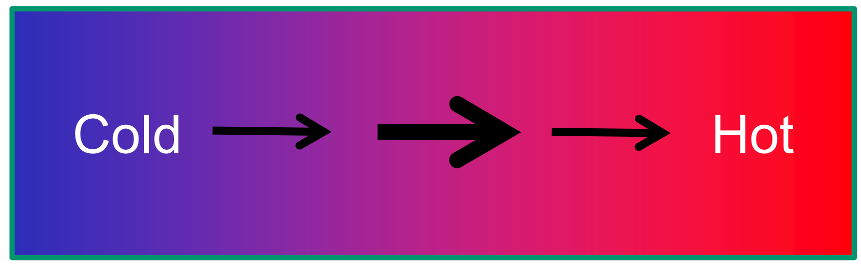
$$\langle u \rangle_* = \frac{\sum_j^S \sum_{i\in C}^{N(t_j)} v_i(t_j)}{\sum_j^S N(t_j)}$$

Anomalous Fluid Velocity

Mean instantaneous fluid velocity measurement gives an anomalous flow in a <u>closed</u> system at steady state with ∇T.

Using the cumulative mean, $\langle u \rangle_*$, gives the expected result of zero fluid velocity.

$$\langle u \rangle = \left\langle \frac{J}{M} \right\rangle \propto x(L-x)\nabla T$$



$$\langle u \rangle_* = \frac{\langle J \rangle}{\langle M \rangle} = 0$$

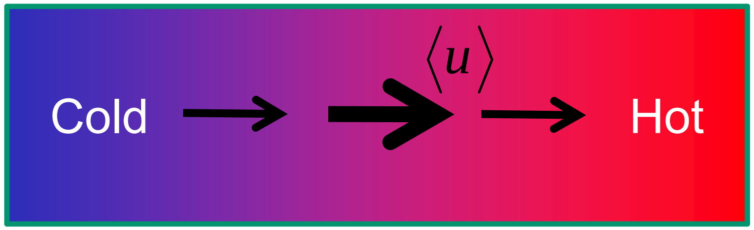
Fluid Velocity & Fluctuations

From the definitions,

$$\langle u \rangle \approx \langle u \rangle_* - \frac{\langle \delta\rho\delta u \rangle}{\langle \rho \rangle}$$

From correlation of non-equilibrium fluctuations,

$$\langle \delta\rho(x)\delta u(x) \rangle \propto -x(L-x)\nabla T$$



This effect is the origin of the anomalous fluid velocity.

M. Tysanner and ALG,
J. Comp. Phys. **196** 173-83 (2004).

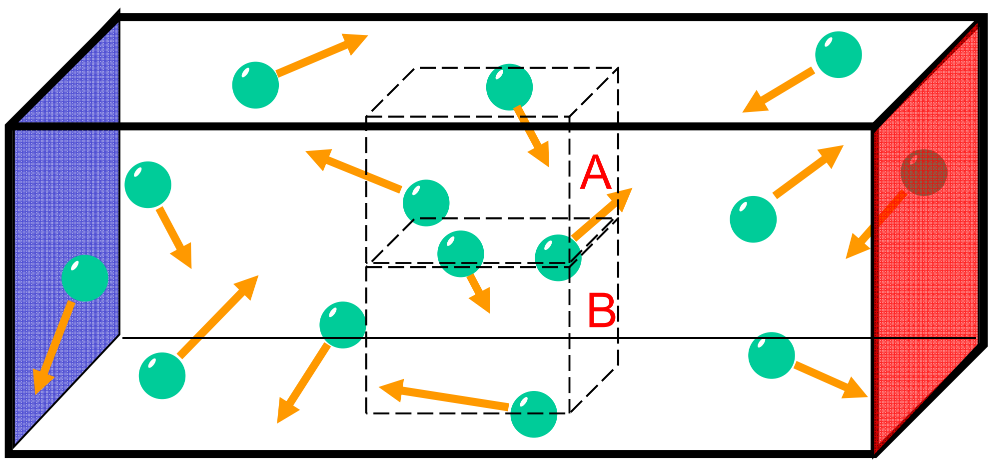
Instantaneous Temperature

Instantaneous temperature has a similar error due to density-temperature correlation of fluctuations.

$$\langle T \rangle \approx \langle T \rangle_* - \frac{\langle \delta\rho \delta T \rangle}{\langle \rho \rangle}$$

Error goes as 1/*N*, so instantaneous temperature is *not* an intensive quantity.

Temperature of cell A = temperature of cell B but *not* equal to temperature of super-cell (A U B)



ALG, *Comm. App. Math. Comp. Sci.* **1** 53-78 (2006)

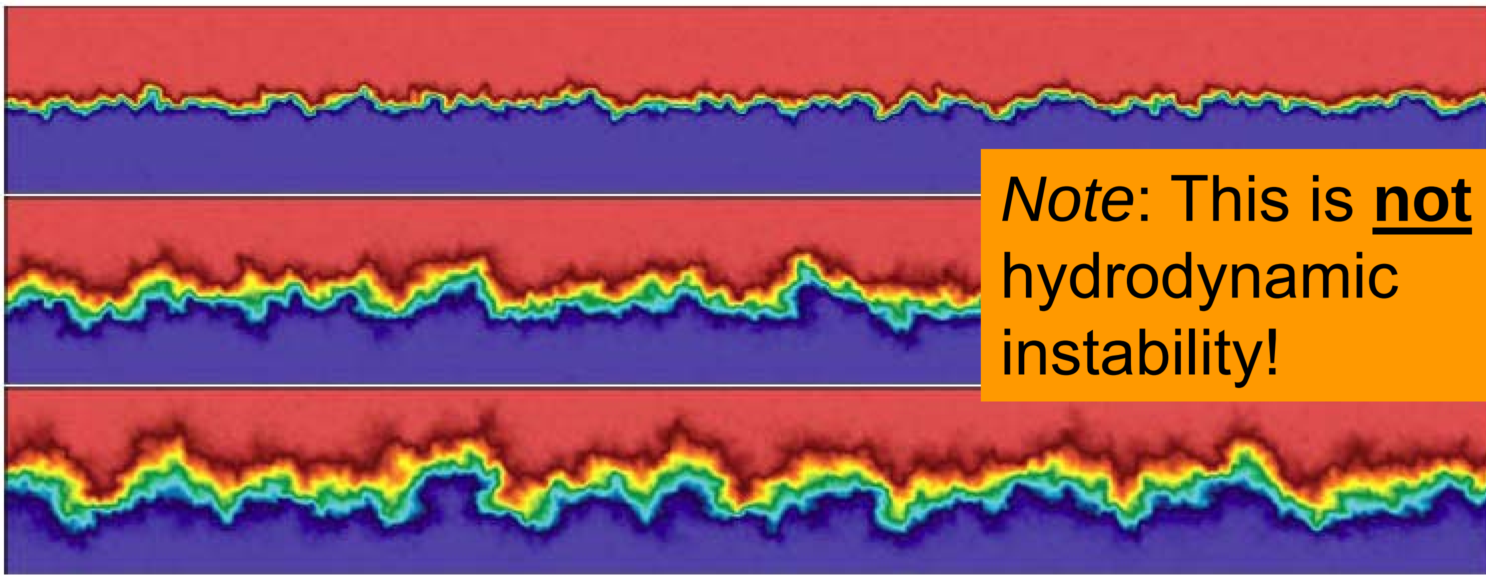
Fluctuation Examples (2)

- Anomalous fluid velocity and temperature in DSMC
- Enhancement of diffusion by fluctuations
- Fluctuations in reaction – diffusion problems

Due to non-equilibrium correlations of fluctuations the effective diffusion coefficient is enhanced and the effect is depends on the size of the system *perpendicular* to the gradient.

Giant Fluctuations in Mixing

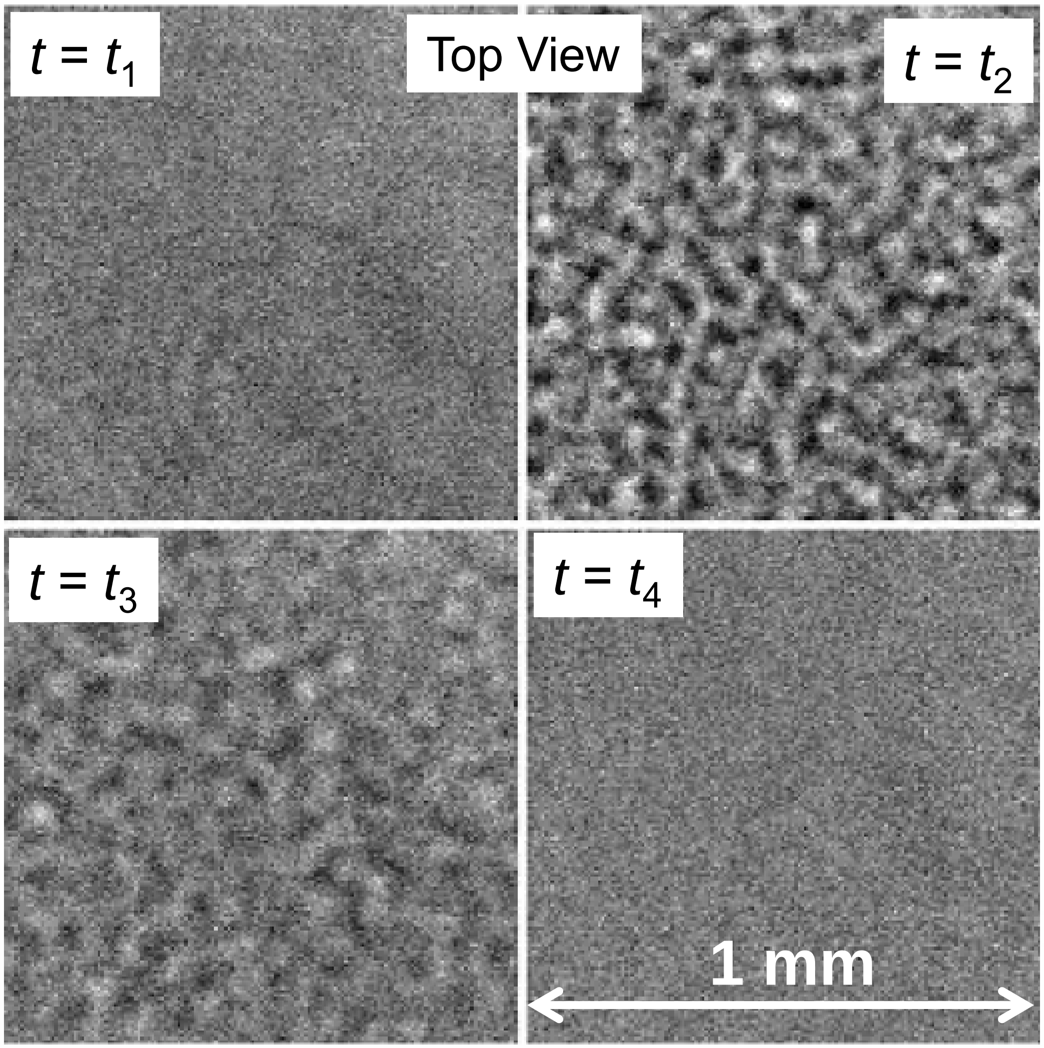
Fluctuations grow large during mixing even when the two species are identical (red & blue).



Note: This is **not** a hydrodynamic instability!

Snapshots of the concentration during the diffusive mixing of two fluids (red and blue) at t = 1 (top), t = 4 (middle), and t = 10 (bottom), starting from a flat interface (phase-separated system) at t = 0.

Experimental Observations

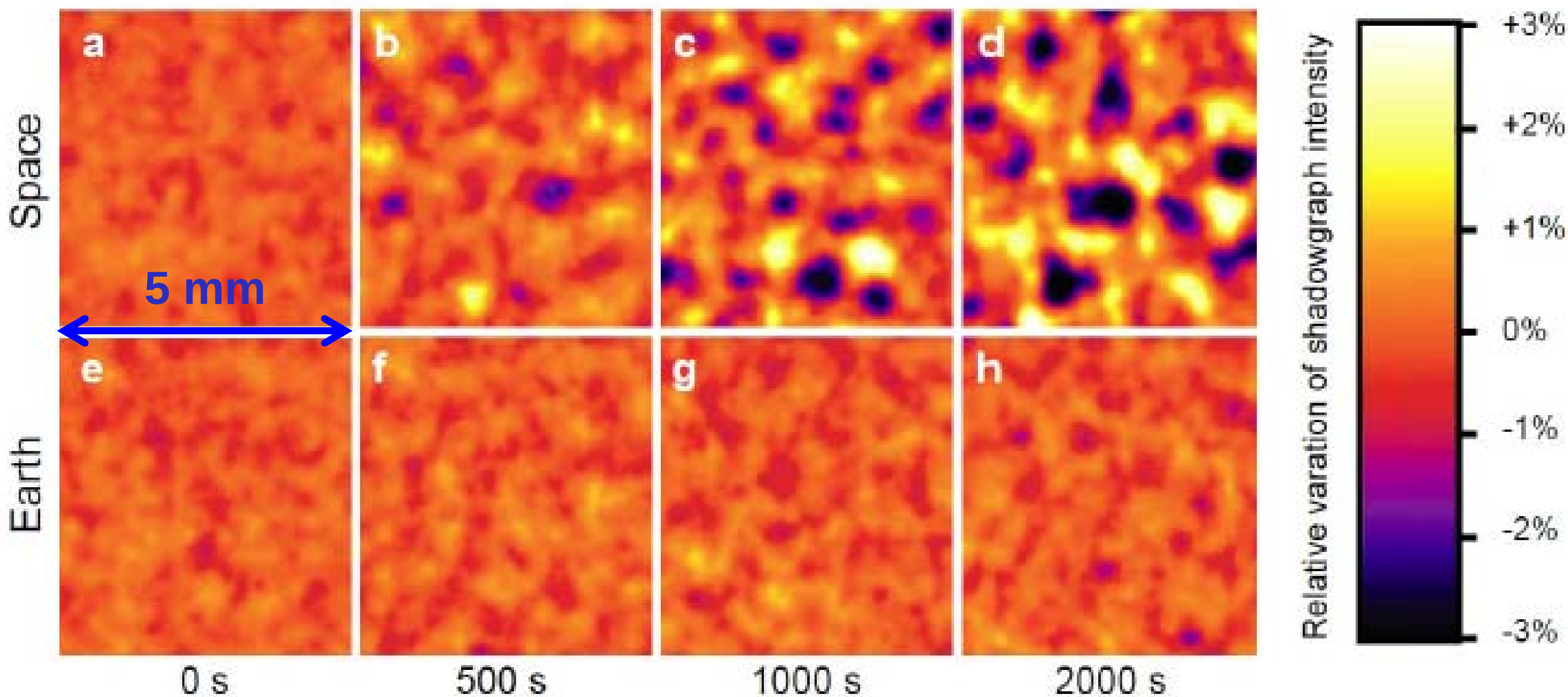


Giant fluctuations in diffusive mixing seen in lab experiments.

Experimental images of interface between two miscible fluids.

Vailati and Giglio, *Nature* 390, 262 (1997).

Experimental Observations (cont.)



Experiments confirm that concentration fluctuations are reduced by gravity with a cut-off wavelength that goes as $1 / g^{1/4}$.

Vailati, et al., Nature Comm., 2:290 (2011).

http://cims.nyu.edu/~donev/FluctHydro/GiantFluct/mixing_grav.mov

Fluctuating Hydrodynamic Theory

Using fluctuating hydrodynamic in the isothermal, incompressible approximation one finds a correlation in the fluctuations of concentration and velocity.

Solving in Fourier space gives the correlation function,

$$\hat{S}_{c,u_\parallel}(\mathbf{k}) = \left\langle \delta\hat{c}\,\delta\hat{u}_\parallel \right\rangle \propto \underline{\nabla} c_0 \;\frac{k_\perp^2}{k^2}$$

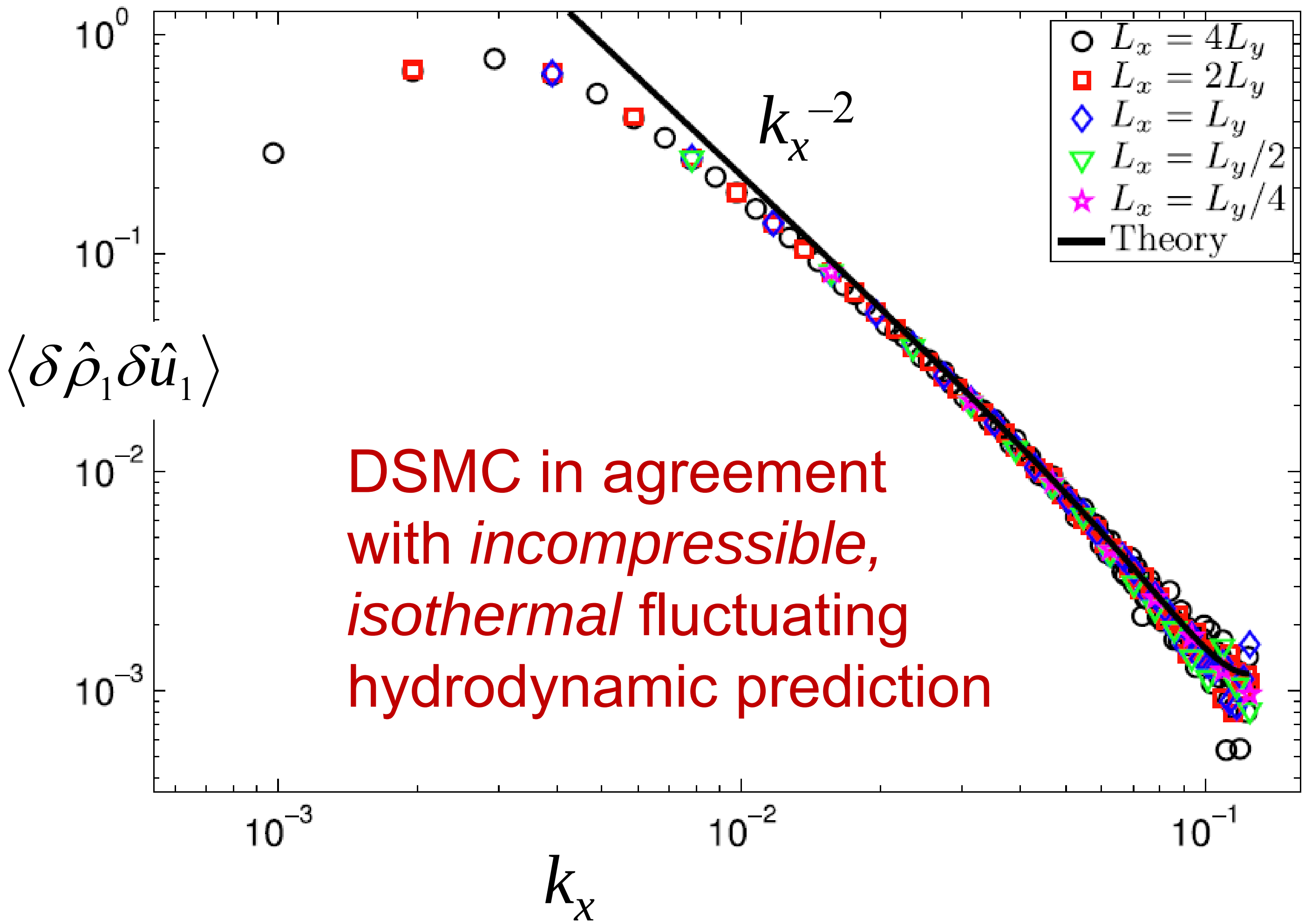
Note: Linear in gradient

Can easily test this prediction using DSMC simulations.

A. Donev, ALG, A. de la Fuente, and J.B. Bell, *J. Stat. Mech.* 2011:P06014 (2011)

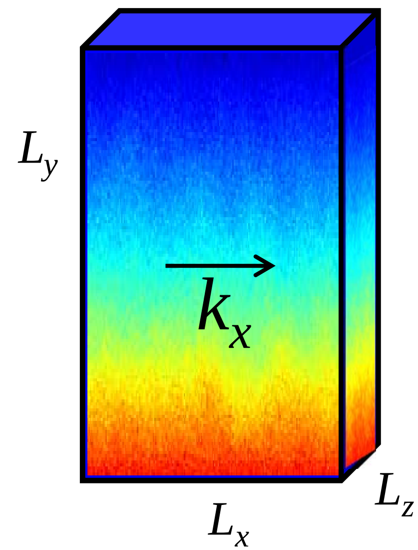
A. Donev, ALG, A. de la Fuente, and J.B. Bell, *Phys. Rev. Lett.*, 106(20): 204501 (2011)

Concentration-Velocity Correlation



DSMC in agreement with *incompressible, isothermal* fluctuating hydrodynamic prediction

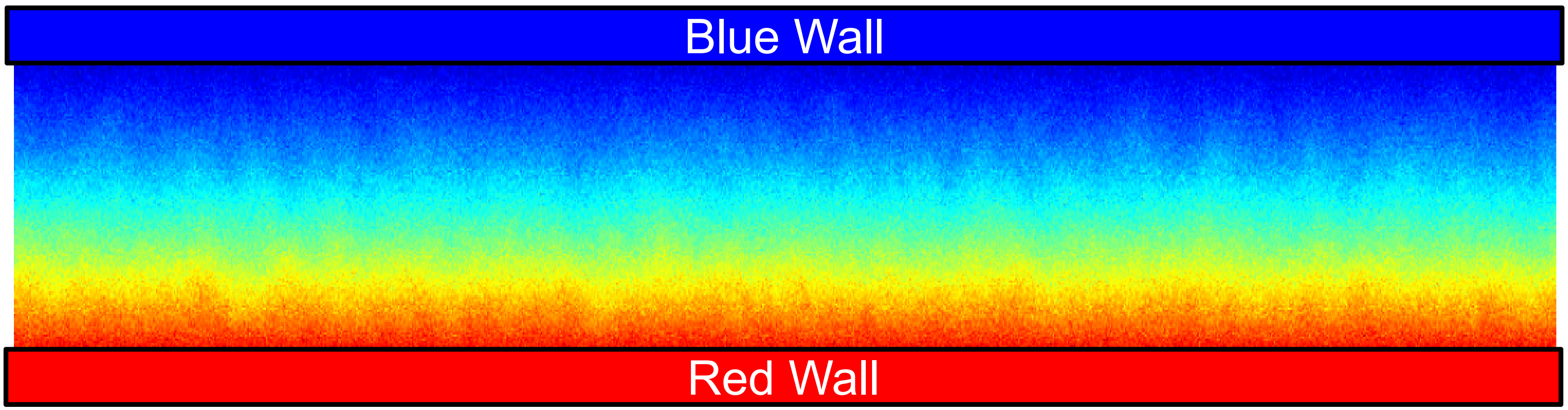
Symbols are DSMC; $k_y = 0$



$L_y = 512\ \lambda;\ L_z = 2\ \lambda$

Diffusion Flux & Fluctuations

Consider a monatomic gas of “red” and “blue” particles with a steady state gradient imposed by wall boundaries.



The non-equilibrium correlation $\left\langle \delta\hat{c}\,\delta\hat{u}_{\parallel} \right\rangle$ enhances the effective flux of concentration even at this steady state.

Fluctuating Hydrodynamics Theory

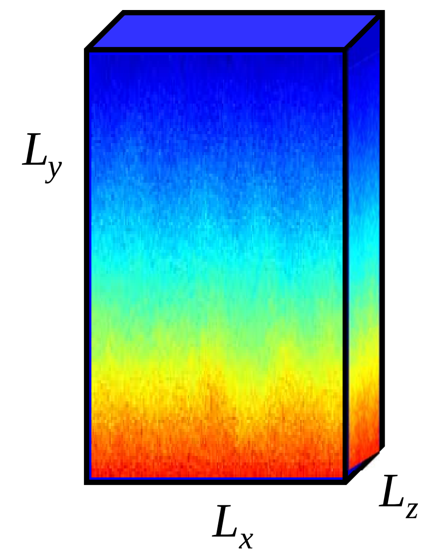
The total mass flux for concentration species is,

$$\left\langle \mathbf{J}_c \right\rangle \approx D_0 \nabla c + \int_k \left\langle \delta \hat{c} \, \delta \hat{\mathbf{u}}_{\parallel} \right\rangle d\mathbf{k} = (D_0 + \Delta D) \nabla c$$

where D_0 is the “bare” diffusion coefficient and the enhancement ΔD is due to correlation of fluctuations.

For a slab geometry $(L_z \ll L_x \ll L_y)$ we have,

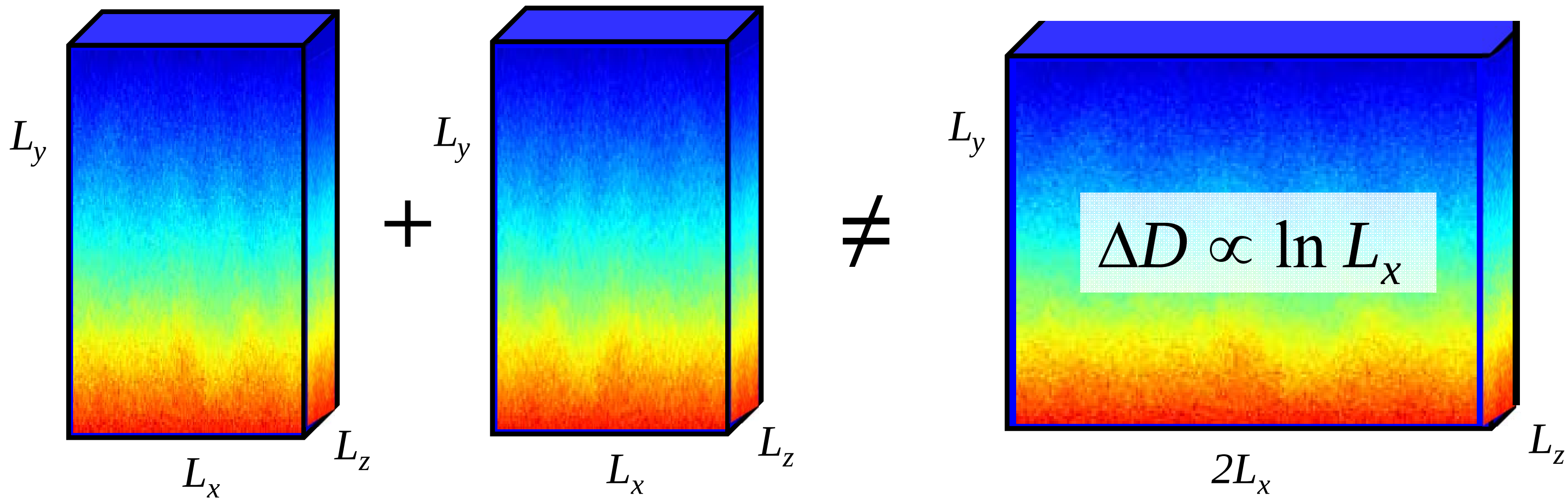
$$\Delta D \approx \frac{k_B T}{4\pi (D_0 + \nu) L_z} \ln \frac{L_x}{L_{mol}}$$



Note: Diffusion enhancement, $\Delta D \propto \ln L_x$

Diffusion and System Geometry

Spectrum of hydrodynamic fluctuations is truncated at wavenumbers given by the size of the physical system.



The wider system can accommodate long wavelength fluctuations, thus it has an enhanced diffusion rate.

Fluctuating Navier-Stokes Solvers

Have simple, accurate, and efficient finite volume schemes for the stochastic PDEs of fluctuating hydrodynamics.

$$U_j^{n+\frac{1}{3}} = U_j^n + \Delta U_j(U^n, W_1) \text{ (estimate at } t = (n+1)\Delta t \text{)}$$

$$U_j^{n+\frac{2}{3}} = \frac{3}{4}U_j^n + \frac{1}{4}\left[U_j^{n+\frac{1}{3}} + \Delta U_j(U_j^{n+\frac{1}{3}}, W_2)\right] \text{ (estimate at } t = (n+\frac{1}{2})\Delta t \text{)}$$

$$U_j^{n+1} = \frac{1}{3}U_j^n + \frac{2}{3}\left[U_j^{n+\frac{2}{3}} + \Delta U_j(U^{n+\frac{2}{3}}, W_3)\right],$$

3rd Order Runge-Kutta

where

$$\underbrace{\Delta U_j(U,W)}_{\text{Change in Mass, Momentum, Energy}} = -\frac{\Delta t}{\Delta x}\left[\underbrace{F_{j+\frac{1}{2}}(U) - F_{j-\frac{1}{2}}(U)}_{\text{Deterministic Flux}}\right] + \frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(\underbrace{Z_{j+\frac{1}{2}} - Z_{j-\frac{1}{2}}}_{\text{Stochastic Flux}}\right).$$

J.B. Bell, ALG, and S. Williams, *Physical Review E* 76 016708 (2007)
A. Donev, E. Vanden-Eijnden, ALG, and J. B. Bell, *CAMCoS*, 5(2):149-197, (2010)

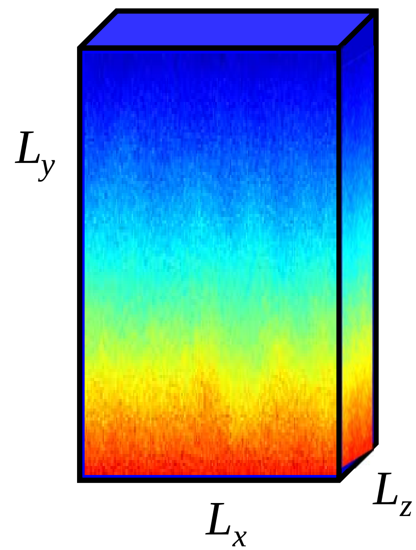
DSMC Measurements

Can separate the contributions to the concentration flux as,

$$\langle \mathbf{J}_1 \rangle = \underbrace{\langle \rho_1 \mathbf{u}_1 \rangle}_{D_{\text{eff}} \nabla c} = \underbrace{\langle \rho_1 \rangle \langle \mathbf{u}_1 \rangle}_{D_0 \nabla c} + \underbrace{\langle \delta\rho_1 \delta\mathbf{u}_1 \rangle}_{\Delta D \nabla c}$$

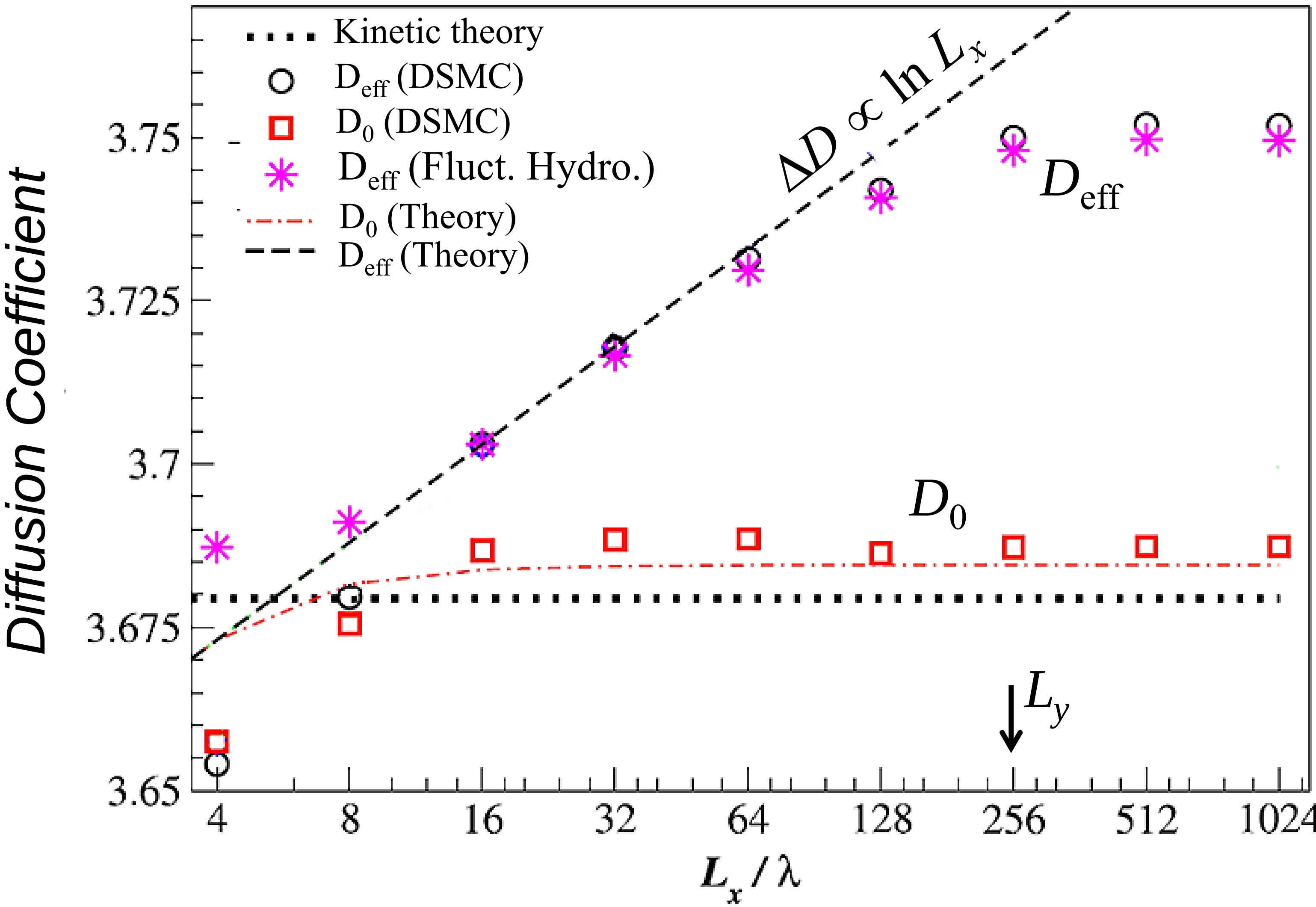
In DSMC we can easily measure

$$\langle \rho_1 \rangle, \langle \mathbf{u}_1 \rangle, \langle \rho_1 \mathbf{u}_1 \rangle \text{ and } \nabla c$$

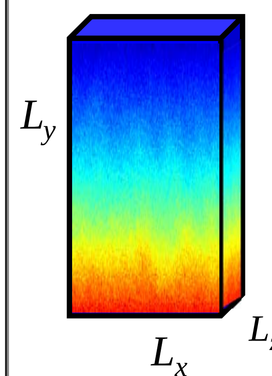


Find the bare diffusion coefficient D_0 and the total effective diffusion coefficient D_{eff}

DSMC and FNS Results (Quasi-2D)

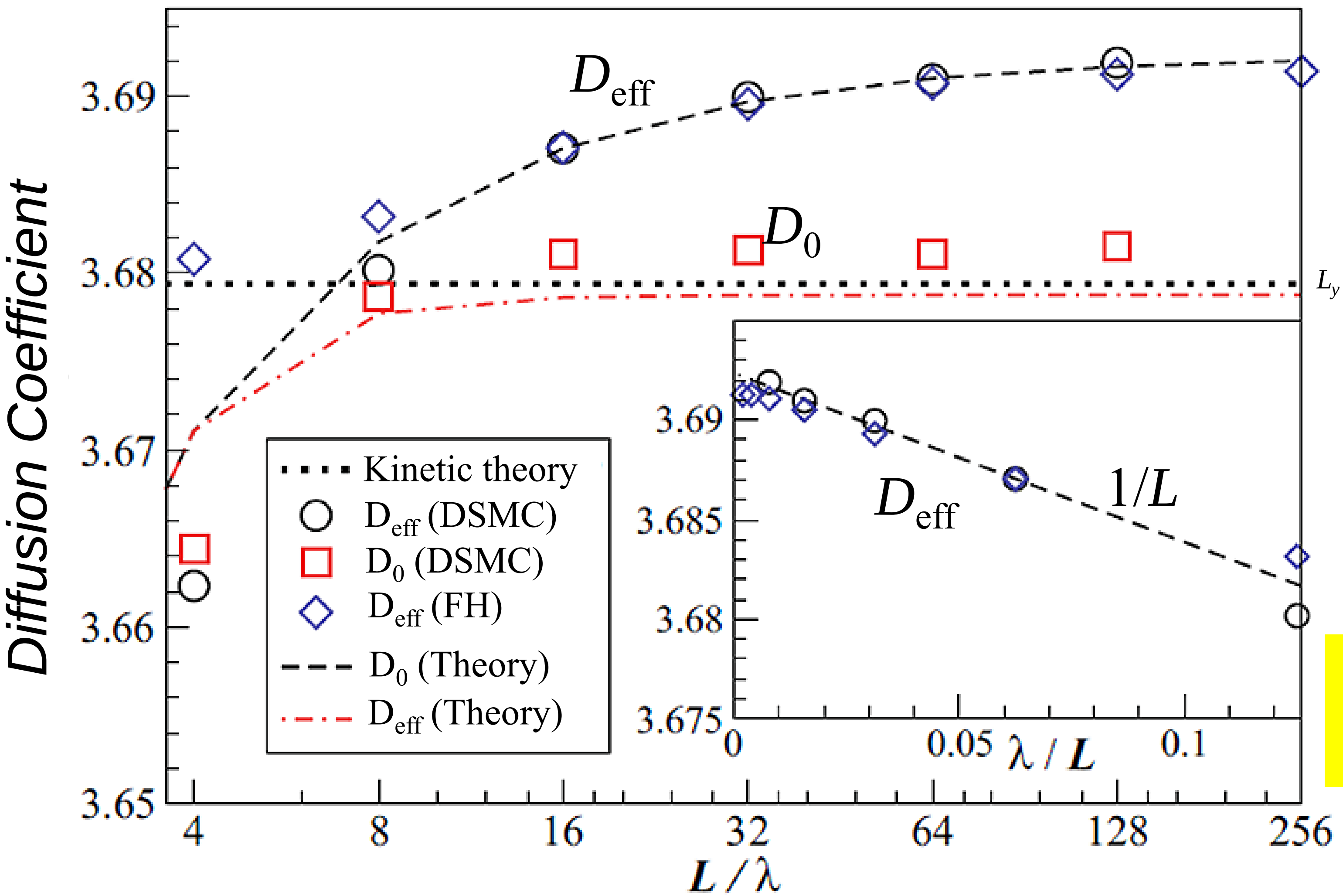


Quasi-2D
($L_z << L_y$)

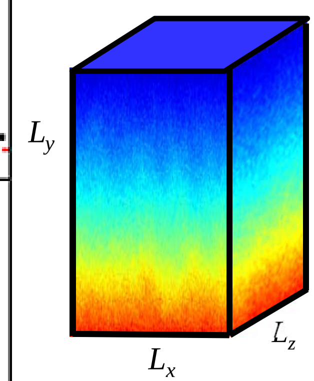


$L_y = 256\ \lambda$
$L_z = 2\ \lambda$

DSMC and FNS Results (Full 3D)



Full 3D
$(L_x = L_z)$



$L_y = L_z = L$

ΔD goes as
$1/L_0 - 1/L$

Fluctuation Examples (3)

- Anomalous fluid velocity and temperature in DSMC
- Enhancement of diffusion by fluctuations
- Fluctuations in reaction – diffusion problems

Study of fluctuating hydrodynamics is being extended to realistic gases, including chemistry.

Realistic Gases

The phenomena in the first two fluctuation examples are present in simple gases, such as the hard sphere model.

Realistic gases introduce additional physical effects:

- Complex transport properties (e.g., Soret effect)
- Internal degrees of freedom
- Disassociation, recombination, and chemistry
- Non-ideal gas equation of state

Both DSMC and fluctuating hydrodynamics become more complicated but interesting new phenomena appear.

Fluctuating Multi-species Fluids

Stochastic PDE for multi-species fluids has the form,

$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla \cdot (\rho \mathbf{u} Y_k) + \underbrace{\nabla \cdot \left[\mathbf{F}_k + \widetilde{\mathbf{F}}_k\right]}_{\text{Diffusion}} = \underbrace{\Omega_k + \widetilde{\Omega}_k}_{\text{Chemistry}}$$

The stochastic species diffusion flux is

$$\widetilde{\mathbf{F}}_k = \sqrt{\rho} \sum_{l=1}^{N_s} L_{kl} \mathbf{W}_k$$

where **W** is a white noise of unit variance.

The matrix $\mathbf{L}$ given by the Cholesky decomposition of a matrix involving the mass fractions Y_k, the molecular weights, and the matrix of diffusion coefficients.

K. Balakrishna, J.B. Bell, ALG. and A. Donev, *28th RGD* Proceedings (2012)

Fluctuating Chemistry

For chemical reaction of the general form,

$$\sum_{k=1}^{N_s} r_{k,l} S_k \xrightarrow{K_l} \sum_{k=1}^{N_s} p_{k,l} S_k \qquad l = 1, \ldots, M_r$$

The deterministic rate of reactions is

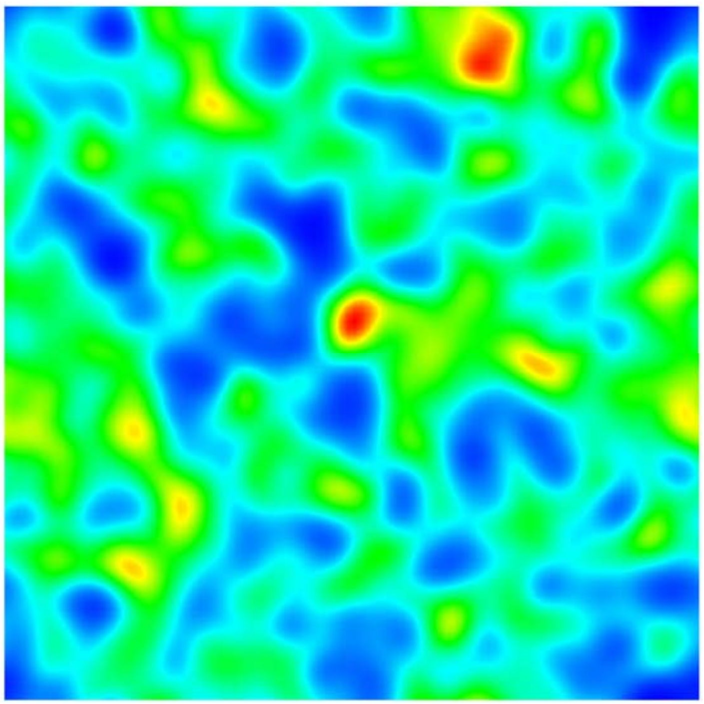
$$\Omega_k = \sum_{l=1}^{M_r} \nu_{k,l} W_k K_l \prod_{i=1}^{N_s} \left(\frac{\rho Y_k}{W_k} \right)^{r_{i,l}} \qquad \nu_{k,l} = p_{k,l} - r_{k,l}$$

and the stochastic rate of reaction is

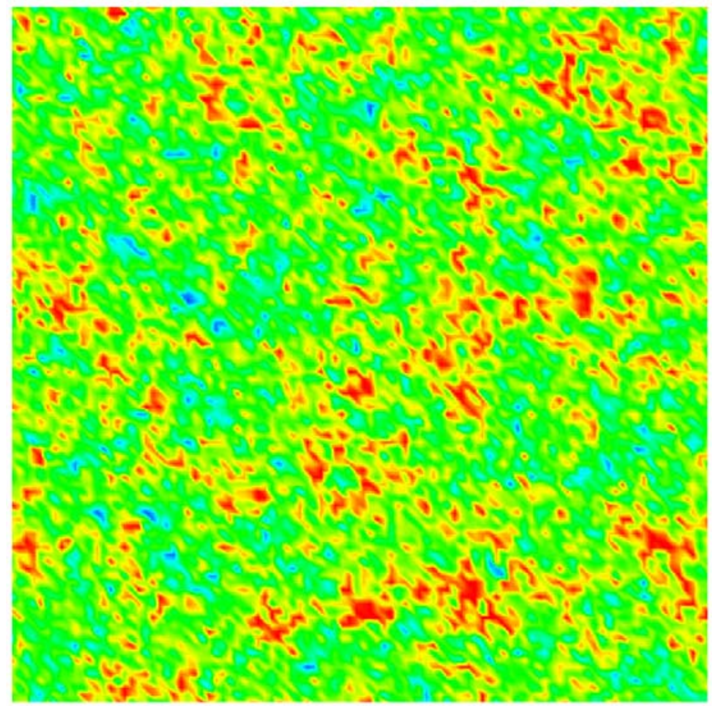
$$\widetilde{\Omega}_k = \sum_{l=1}^{M_r} \nu_{k,l} W_k \sqrt{\frac{K_l}{N_A} \prod_{i=1}^{N_s} \left(\frac{\rho Y_k}{W_k} \right)^{r_{i,l}}} \, \mathrm{W}_l$$

Turing Pattern Instability

Fluctuations change the Turing instability patterns in reaction – diffusion simulations of Brusselator model



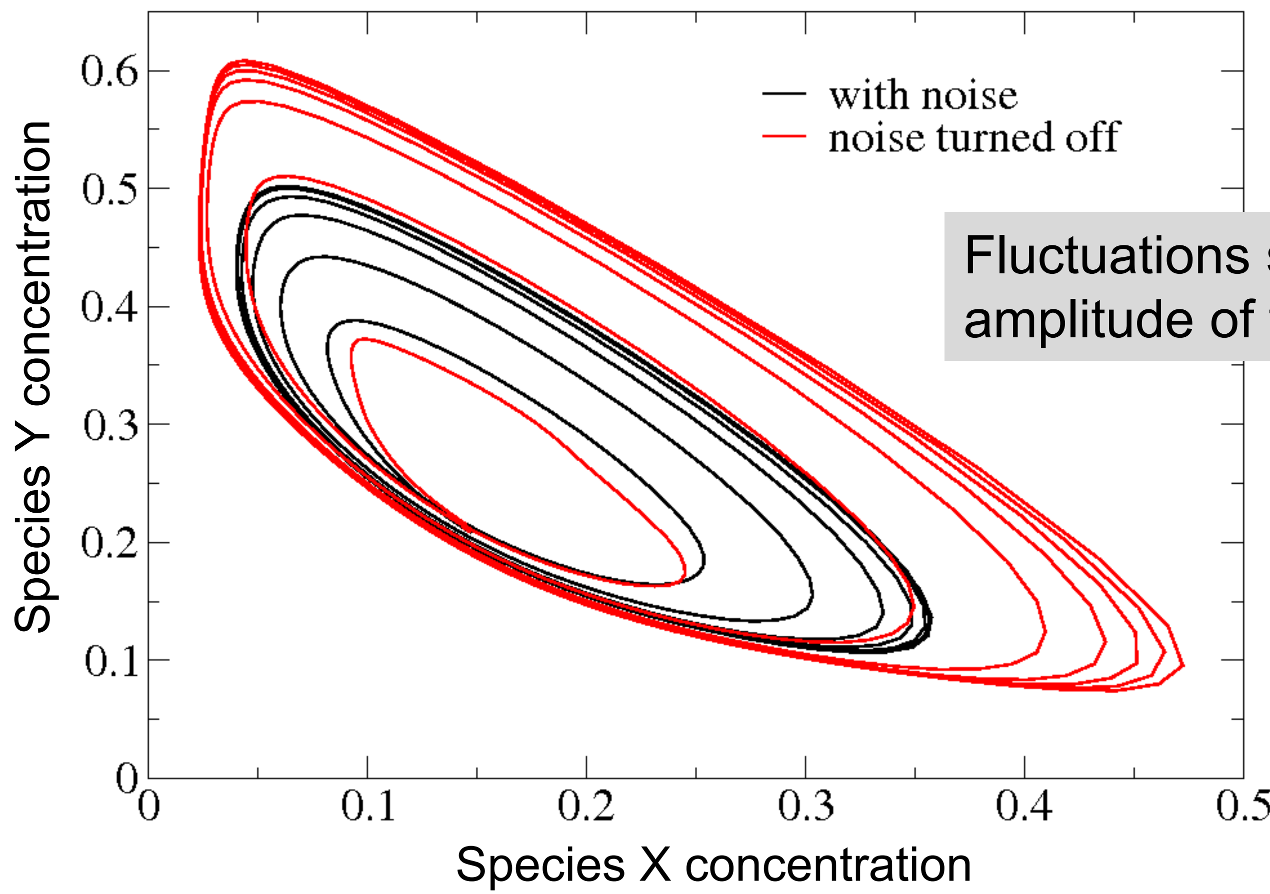
Deterministic hydrodynamics and chemistry



Fluctuating hydrodynamics and chemistry

Turing Instability Limit Cycle

Spatially-averaged concentrations of X and Y vary in time as a limit cycle.



Fluctuations suppress the amplitude of the cycle.

Future Work

- Developing incompressible and low-Mach number schemes for fluctuating hydrodynamics

- Extensions to complex fluids (e.g., Cahn-Hilliard)

- Exploring DSMC / FNS hybrids using Adaptive Mesh and Algorithm Refinement

For more information, visit:
www.algarcia.org, cse.lbl.gov
and cims.nyu.edu/~donev

Supported
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DSMC 2013 Workshop

Late September 2013
Hosted by Sandia Lab.

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