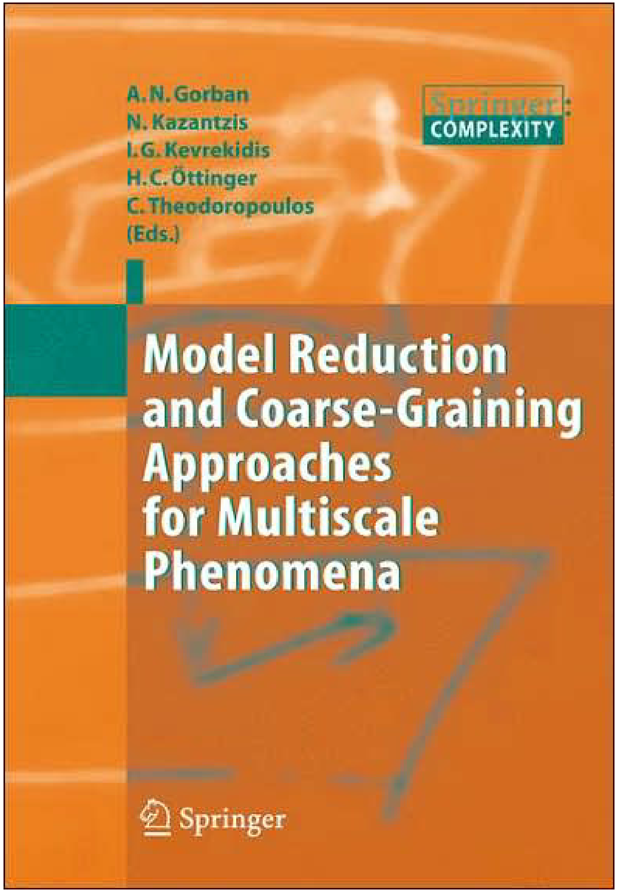
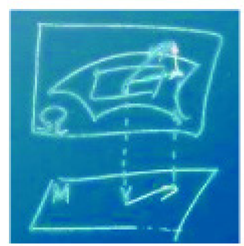


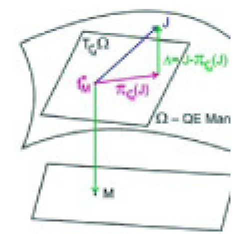
How About Coarse Graining???

siam · University of Leicester · Warwick Mathematics Institute WMI · MANCHESTER 1824

Mathematics of Model Reduction



Research Workshop
University of Leicester, UK
August 28-30, 2007
Att LT3



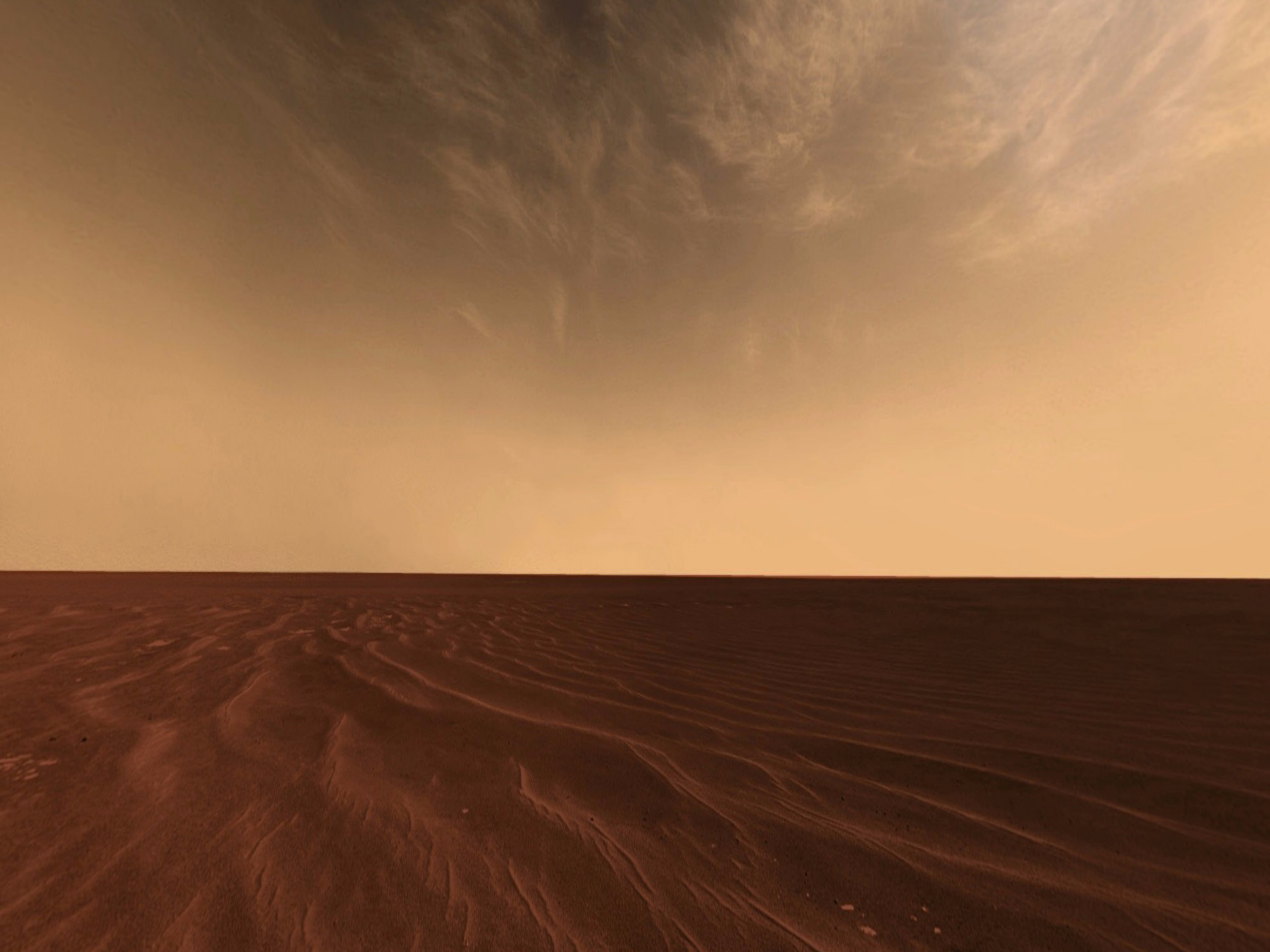
Joint workshop with SIAM, supported by LMS

Fluctuation Renormalization and Mode Coupling

More Questions than Answers?!

Hans Christian Öttinger

Department of Materials, ETH Zürich, Switzerland




BikeCam.ch

GENERIC Structure

General equation for the nonequilibrium reversible-irreversible coupling

metriplectic structure (P. J. Morrison, 1986)

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x}$$

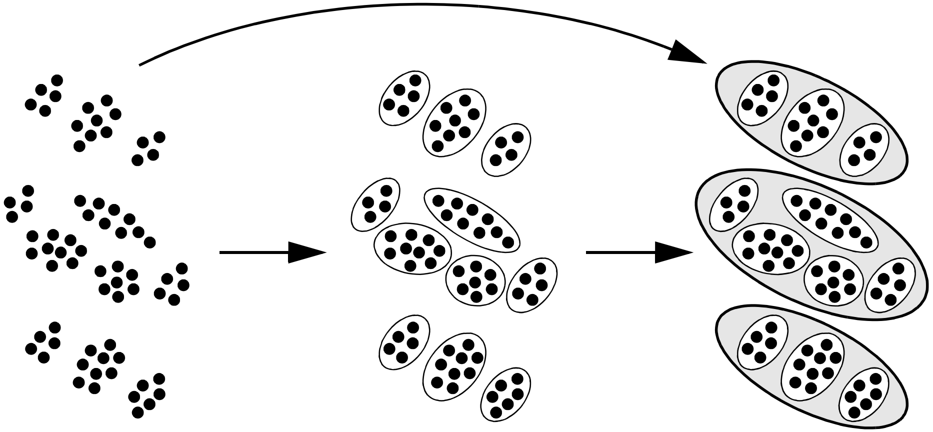
$$L(x) \cdot \frac{\delta S(x)}{\delta x} = 0$$

L antisymmetric, Jacobi identity

$$M(x) \cdot \frac{\delta E(x)}{\delta x} = 0$$

M Onsager/Casimir symm., positive-semidefinite

Statistical Mechanics: Entropy



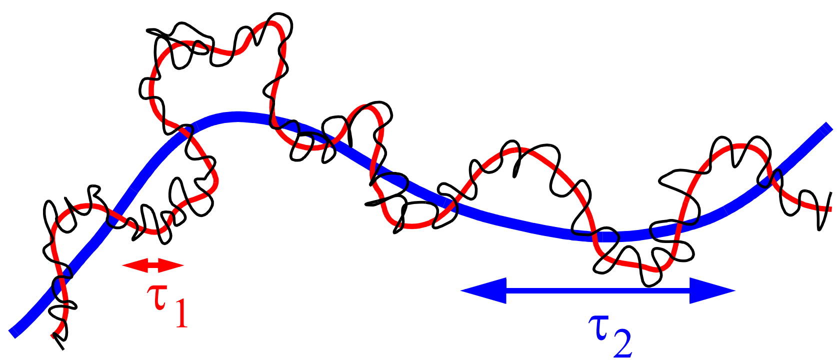
relative entropy

Statistical Mechanics: Friction Matrix

$$M_{jk} = \frac{1}{k_B}\int_0^{\tau} \langle \dot{\Pi}^{f}_{k}(0)\dot{\Pi}^{f}_{j}(t)\rangle_x dt$$ Green-Kubo

$$M_{jk} = \frac{1}{2k_B\tau}\langle \Delta_\tau \Pi_j \, \Delta_\tau \Pi_k \rangle_x$$ Einstein

cf. $D = \frac{1}{2\Delta t}\langle (\Delta x)^2 \rangle$



MULTISCALE MODEL. SIMUL.
Vol. 6, No. 1, pp. 53–69

THE MATHEMATICAL PROCEDURE OF COARSE GRAINING: FROM GRAD'S TEN-MOMENT EQUATIONS TO HYDRODYNAMICS*

HANS CHRISTIAN ÖTTINGER† AND HENNING STRUCHTRUP‡

Abstract. We employ systematic coarse graining techniques to derive hydrodynamic equations from Grad's ten-moment equations. The coarse graining procedure is designed such that it manifestly preserves the thermodynamic structure of the equations. The relevant thermodynamic structure and the coarse graining recipes suggested by statistical mechanics are described in detail and are illustrated by the example of hydrodynamics. A number of mathematical challenges associated with structure-preserving coarse graining of evolution equations for thermodynamic systems as a generalization of Hamiltonian dynamic systems are presented. Coarse graining is a key step that should always be considered before attempting to solve an equation.

Key words. coarse graining, dynamic systems, Poisson brackets, dissipative brackets, general equation for the nonequilibrium reversible-irreversible coupling structure, nonequilibrium thermodynamics, hydrodynamics, Grad's moment equations

GENERIC with Fluctuations

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x} + B(x) \cdot \frac{dW_t}{dt} + k_\mathrm{B} \frac{\delta}{\delta x} \cdot M(x)$$

Itô

$$B(x) \cdot B(x)^T = 2 k_\mathrm{B} M(x)$$

fluctuation-dissipation theorem

$$\left\langle \frac{dW_t}{dt} \right\rangle = 0 \qquad \left\langle \frac{dW_t}{dt} \frac{dW_{t'}}{dt'} \right\rangle = \delta(t - t') \mathbf{1}$$

Wiener process

Some important issues:

- Partial stochastic differential equations
- Fluctuation renormalization (long-time tails, mode-coupling)

Fluctuation Renormalization

$$\frac{dx}{dt} = L(x) \cdot \frac{\delta E(x)}{\delta x} + M(x) \cdot \frac{\delta S(x)}{\delta x} + B(x) \cdot \frac{dW_t}{dt} + k_B \frac{\delta}{\delta x} \cdot M(x)$$

- Elimination of noise by coarse graining operation
- Projections from probability distributions to averages
- Warning about time scales: Onsager's regression hypothesis
- Renormalized friction matrix $M(x)$

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$$\mu_{jk}(t) = \frac{1}{k_B} \sum_{l,l'} \langle \hat{\varphi}_l \dot{x}_k \rangle_{\bar{x}} \, [e^{A(\bar{x})t}]_{ll'} \, \langle \hat{\varphi}_{l'} \dot{x}_j \rangle_{\bar{x}}$$

$\hat{\varphi}_l$: ON basis of orthogonal complement to space of linear functions

$$A_{ll'}(\bar{x}) = \langle \hat{\varphi}_l \, \mathcal{L} \hat{\varphi}_{l'} \rangle_{\bar{x}}$$

$\mathcal{L}$: infinitesimal generator of FPE

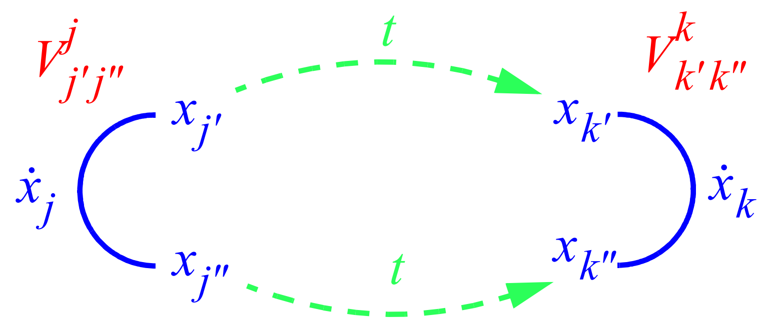
Mode Coupling

- Only quadratic functions
- Only Gaussian fluctuations
- Only drift term of infinitesimal generator

$$\mu_{jk}(t) = \frac{1}{2k_B} \sum_{j'j''k'k''} \frac{\delta^2 \dot{x}_k(\bar{x})}{\delta\bar{x}_{k'}\delta\bar{x}_{k''}} [C(\bar{x}) \cdot e^{a(\bar{x})t}]_{k'j'} [C(\bar{x}) \cdot e^{a(\bar{x})t}]_{k''j''} \frac{\delta^2 \dot{x}_j(\bar{x})}{\delta\bar{x}_{j'}\delta\bar{x}_{j''}}$$

$$C(\bar{x}) = \langle (x-\bar{x})(x-\bar{x}) \rangle_{\bar{x}}$$

$$a_{jk}(\bar{x}) = \frac{\delta \dot{x}_k(\bar{x})}{\delta \bar{x}_j}$$



Remarks

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- Manageable calculations (use eigenmodes!)

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Remarks (Continued)

- Manageable calculations (use eigenmodes!)
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- How about energy conservation?

Remarks (Continued)

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- How about energy conservation? It suggests:
- $$\frac{\delta^2 \dot{x}_j^{\text{rev}}}{\delta\bar{x}_{j'}\delta\bar{x}_{j''}} = \frac{\delta^2 L_{jk}}{\delta\bar{x}_{j'}\delta\bar{x}_{j''}} \frac{\delta E}{\delta x_k}$$

Fluctuation Renormalization: Summary

- What is the problem?
- What do we get from projection-operator techniques?
- How can we use mode coupling theory?
- Is there any objective result?
- Are there distinguished variables? (universal or problem-specific?)
- Are Lie-Poisson brackets the key?
- How about energy conservation for the renormalized theory?

$$V^{j}_{j'j''} = \frac{\delta^2 L_{jk}}{\delta\bar{x}_{j'}\delta\bar{x}_{j''}} \frac{\delta E}{\delta x_k}$$