How About Coarse Graining???
Fluctuation Renormalization and Mode Coupling

More Questions than Answers?!

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**GENERIC Structure**

General equation for the nonequilibrium reversible-irreversible coupling metriplectic structure (P. J. Morrison, 1986)

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

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

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

\( L \) antisymmetric, Jacobi identity

\( M \) Onsager/Casimir symm., positive-semidefinite
Statistical Mechanics: Entropy

relative entropy
Statistical Mechanics: Friction Matrix

\[
M_{jk} = \frac{1}{k_B} \int_0^\tau \left\langle \Pi_k(0) \Pi_j(t) \right\rangle_x dt \quad \text{Green-Kubo}
\]

\[
M_{jk} = \frac{1}{2k_B \tau} \left\langle \Delta_\tau \Pi_j \Delta_\tau \Pi_k \right\rangle_x \quad \text{Einstein}
\]

\[
f \quad \text{cf. } D = \frac{1}{2\Delta t} \left\langle (\Delta x)^2 \right\rangle
\]
THE MATHEMATICAL PROCEDURE OF COARSE GRAINING: FROM GRAD'S TEN-MOMENT EQUATIONS TO HYDRODYNAMICS*

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

\[
B(x) \cdot B(x)^T = 2k_B M(x)
\]

fluctuation-dissipation theorem

\[
\langle \frac{dW_t}{dt} \rangle = 0 \quad \langle \frac{dW_t}{dt} \frac{dW_{t'}}{dt'} \rangle = \delta(t-t') \cdot 1
\]

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 \( M(x) \)
Fluctuation Renormalization

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- Elimination of noise by coarse graining operation
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\[
\mu_{jk}(t) = \frac{1}{k_B} \sum_{l, l'} \langle \hat{\phi}_l \dot{x}_k \rangle_{\bar{x}} [ e^{A(\bar{x})t} ]_{ll'} \langle \hat{\phi}_{l'} \dot{x}_j \rangle_{\bar{x}} \quad \hat{\phi}_l : \text{ON basis of orthogonal complement to space of linear functions}
\]

\[
A_{ll'}(\bar{x}) = \langle \hat{\phi}_l \hat{\phi}_{l'} \rangle_{\bar{x}} \quad \mathcal{K} : \text{infinitesimal generator of FPE}
\]
Mode Coupling

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

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

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

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

- Manageable calculations (use eigenmodes!)
\[ \mu_{jk}(t) = \frac{1}{2k_B} \sum_{j'j''k'k''} \frac{\delta^2 \dot{x}_k(\bar{x})}{\delta \bar{x}_{k'}, \delta \bar{x}_{k''}} \left[ C(\bar{x}) \cdot e^{a(\bar{x})t} \right]_{k'j'} \left[ C(\bar{x}) \cdot e^{a(\bar{x})t} \right]_{k''j''} \frac{\delta^2 \dot{x}_j(\bar{x})}{\delta \bar{x}_{j'}, \delta \bar{x}_{j''}} \]

- Manageable calculations (use eigenmodes!)
- Use reversible contribution to \( \frac{\delta^2 \dot{x}_j(\bar{x})}{\delta \bar{x}_{j'}, \delta \bar{x}_{j''}} \) only (GK: linear superposition of noise on different scales)
$\mu_{jk}(t) = \frac{1}{2k_B} \sum_{j'j''k'k''} \frac{\delta^2 \dot{x}_k(\bar{x})}{\delta \bar{x}_{k'} \delta \bar{x}_{k''}} \left[ C(\bar{x}) \cdot e^{a(\bar{x}) t} \right]_{k'j'} [C(\bar{x}) \cdot e^{a(\bar{x}) t}]_{k''j''} \frac{\delta^2 \dot{x}_j(\bar{x})}{\delta \bar{x}_{j'} \delta \bar{x}_{j''}}$

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- Use reversible contribution to $\delta^2 \dot{x}_j(\bar{x})/\delta \bar{x}_{j'} \delta \bar{x}_{j''}$ only (GK: linear superposition of noise on different scales)
- No objectivity (under nonlinear transformations of variables!)
\[ \mu_{jk}(t) = \frac{1}{2k_B} \sum_{j'j''k'k''} \frac{\delta^2 x_k(\bar{\xi})}{\delta \bar{\xi}_{k'} \delta \bar{\xi}_{k''}} \left[ C(\bar{\xi}) \cdot e^{a(\bar{\xi})t} \right]_{k'j'} \left[ C(\bar{\xi}) \cdot e^{a(\bar{\xi})t} \right]_{k''j''} \frac{\delta^2 \dot{x}_j(\bar{\xi})}{\delta \bar{\xi}_{j'} \delta \bar{\xi}_{j''}} \]

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- Lack of objectivity is NOT a problem of mode coupling
Remarks

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

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- Lie-Poisson: \( \dot{x}_j^{\text{rev}} = L_{jk} \delta E/\delta x_k = \Gamma^j_{lk} x_l \delta E/\delta x_k \)
Remarks

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\[ \frac{\delta^2 \dot{x}_j^{\text{rev}}}{\delta \bar{x}_{j'} \delta \bar{x}_{j''}} = \Gamma_{jk'}^{j'} \frac{\delta^2 E}{\delta \bar{x}_{j''} \delta \bar{x}_k} + \Gamma_{jk''}^{j''} \frac{\delta^2 E}{\delta \bar{x}_{j'} \delta \bar{x}_k} + \Gamma_{lk}^{jk} x_l \frac{\delta^3 E}{\delta \bar{x}_{j'} \delta \bar{x}_{j''} \delta \bar{x}_k} \]
Remarks (Continued)

- Manageable calculations (use eigenmodes!)
- Use reversible contribution to \( \delta^2 \dot{x}_j(\bar{x}) / \delta \bar{x}_j, \delta \bar{x}_j'' \) only
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\]

- How about energy conservation?
Remarks (Continued)

- Manageable calculations (use eigenmodes!)
- Use reversible contribution to $\delta^2 \dot{x}_j(\bar{x})/\delta \bar{x}_j, \delta \bar{x}_j''$ only
- No objectivity (under nonlinear transformations of variables!)
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- Is there a distinguished linear space of variables?
- Lie-Poisson: $\dot{x}_j^{\text{rev}} = L_{jk} \delta E/\delta x_k = \Gamma^j_{lk} x_l \delta E/\delta x_k$

$$
\frac{\delta^2 \dot{x}_j^{\text{rev}}}{\delta \bar{x}_j', \delta \bar{x}_j''} = \Gamma^j_{jk} \frac{\delta^2 E}{\delta \bar{x}_j' \delta \bar{x}_k} + \Gamma^j_{jk} \frac{\delta^2 E}{\delta \bar{x}_j' \delta \bar{x}_k} + \Gamma^j_{lk} x_l \frac{\delta^3 E}{\delta \bar{x}_j' \delta \bar{x}_j'' \delta \bar{x}_k}
$$

- 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?

\[
V^j_{j'j''} = \frac{\delta^2 L_{jk}}{\delta \dot{x}_{j'} \delta \ddot{x}_{j''}} \frac{\delta E}{\delta x_k}
\]