Problem reduction, memory and renormalization

Panos Stinis

Northwest Institute for Advanced Computing
Pacific Northwest National Laboratory

A simple example

The linear differential system for $x(t)$ and $y(t)$ given by

$$\frac{dx}{dt} = x + y, \;\; x(0) = x_0$$
$$\frac{dy}{dt} = -y + x, \;\; y(0) = y_0$$

can be reduced into an equation for $x(t)$ alone.

$$\frac{dx}{dt} = x + \int_0^t e^{-(t-s)} x(s) ds + y_0 e^{-t}$$

Reduction leads to memory effects

We want a formalism which allows us to generalize this observation to nonlinear systems of arbitrary (but finite) dimension.

A simple example

The linear differential system for $x(t)$ and $y(t)$ given by

$$\frac{dx}{dt} = x + y, \;\; x(0) = x_0$$
$$\frac{dy}{dt} = -y + x, \;\; y(0) = y_0$$

can be reduced into an equation for $x(t)$ alone.

$$\frac{dx}{dt} = x + \int_0^t e^{-(t-s)} x(s) ds + y_0 e^{-t}$$

Reduction leads to memory effects

We want a formalism which allows us to generalize this observation to nonlinear systems of arbitrary (but finite) dimension.

The Mori-Zwanzig formalism

Zwanzig(1961), Mori(1965), Chorin, Hald, Kupferman (2000)

Suppose we are given an M-dimensional system of ordinary differential equations

$$\frac{d\phi(u_0,t)}{dt} = R(\phi(u_0,t)) \tag{1}$$

with initial condition $\phi(u_0,0) = u_0$.

Transform into a system of linear partial differential equations

$$\frac{\partial}{\partial t} e^{tL} u_{0k} = L e^{tL} u_{0k},\ k = 1,\ldots,M$$

where the Liouvillian operator $L = \sum_{i=1}^{M} R_i(u_0)\frac{\partial}{\partial u_{0i}}$. Note that $Lu_{0j} = R_j(u_0)$.

Derivation of the Liouville equation

Let $g(u_0)$ be any (smooth) function of u_0 and define $u(u_0, t) = g(\phi(u_0, t))$.

We now proceed to derive a PDE satisfied by $u(u_0, t)$.

$$\frac{\partial}{\partial t}(u(u_0, t)) = \sum_i (\frac{\partial g}{\partial u_{0i}})(\phi(u_0, t))\frac{\partial}{\partial t}(\phi_i(u_0, t))$$

$$= \sum_i R_i(\phi(u_0, t))(\frac{\partial g}{\partial u_{0i}})(\phi(u_0, t)). \tag{2}$$

We now want to prove that

$$\sum_i R_i(\phi(u_0, t))(\frac{\partial g}{\partial u_{0i}})(\phi(u_0, t)) = \sum_i R_i(u_0)\frac{\partial}{\partial u_{0i}}(g(\phi(u_0, t))). \tag{3}$$

First we prove the following useful identity

$$R(\phi(u_0, t)) = D_{u_0}\phi(u_0, t)R(u_0). \tag{4}$$

In this formula $D_{u_0}\phi(u_0, t)$ is the Jacobian of $\phi(u_0, t)$ and multiplication on the right hand side is a matrix vector multiplication.

Define $F(u_0, t)$ to be the difference of the left hand side and the right hand side of (4)

$$F(u_0, t) = R(\phi(u_0, t)) - D_{u_0}\phi(u_0, t)R(u_0). \tag{5}$$

Then at $t = 0$ we have

$$\begin{aligned} F(u_0, 0) &= R(\phi(u_0, 0)) - D_{u_0}\phi(u_0, 0)R(u_0) && (6)\\ &= R(u_0) - D_{u_0}(u_0) \cdot R(u_0) \\ &= R(u_0) - I \cdot R(u_0) \equiv 0. && (7) \end{aligned}$$

Differentiating F with respect to t we get

$$\frac{\partial}{\partial t}F(u_0,t) = \frac{\partial}{\partial t}R(\phi(u_0,t)) - \frac{\partial}{\partial t}(D_{u_0}\phi(u_0,t)R(u_0)) =$$
$$= \frac{\partial}{\partial t}R(\phi(u_0,t)) - (\frac{\partial}{\partial t}(D_{u_0}\phi(u_0,t)))R(u_0)$$
$$= (D_{u_0}R)(\phi(u_0,t)) \cdot \frac{\partial}{\partial t}\phi(u_0,t) - (D_{u_0}(\frac{\partial}{\partial t}\phi(u_0,t)))R(u_0)$$
$$= (D_{u_0}R)(\phi(u_0,t)) \cdot \frac{\partial}{\partial t}\phi(u_0,t) - (D_{u_0}(R(\phi(u_0,t)))) \cdot R(u_0)$$
$$= (D_{u_0}R)(\phi(u_0,t)) \cdot R(\phi(u_0,t))$$
$$-(D_{u_0}R)(\phi(u_0,t)) \cdot D_{u_0}\phi(u_0,t) \cdot R(u_0)$$
$$= (D_{u_0}R)(\phi(u_0,t)) \cdot [R(\phi(u_0,t)) - D_{u_0}\phi(u_0,t) \cdot R(u_0)]$$
$$= (D_{u_0}R)(\phi(u_0,t)) \cdot F(u_0,t). \qquad (8)$$

From (7) and (8) above we conclude that $F(u_0,t) \equiv 0$. But $F(u_0,t) \equiv 0$ implies (4).

We now use (4) to establish (3). Indeed

$$\sum_i R_i(\phi(u_0,t))(\frac{\partial g}{\partial u_{0i}})(\phi(u_0,t)) =$$

$$= \sum_i (\sum_j \frac{\partial \phi_i}{\partial u_{0j}}(u_0,t) R_j(u_0))(\frac{\partial g}{\partial u_{0i}})(\phi(u_0,t)) =$$

$$= \sum_j R_j(u_0)(\sum_i (\frac{\partial g}{\partial u_{0i}})(\phi(u_0,t))\frac{\partial \phi_i}{\partial u_{0j}}(u_0,t)) =$$

$$= \sum_j R_j(u_0)\frac{\partial}{\partial u_{0j}}(g(\phi(u_0,t))) \qquad (9)$$

The first equality above follows from (4).

From (2) and (3) we conclude that $u(u_0, t)$ solves

$$\begin{cases} \frac{\partial}{\partial t} u(u_0, t) = \sum_j R_j(u_0) \frac{\partial}{\partial u_{0j}} u(u_0, t) = Lu(u_0, t) \\ u(u_0, 0) = g(u_0) \end{cases} \tag{10}$$

where L is the linear differential operator $L = \sum_i R_i(u_0) \frac{\partial}{\partial u_{0i}}$.

Define the evolution operator e^{tL} as follows:

$$\left(e^{tL} g\right)(u_0) = g\left(u(u_0, t)\right)$$

For $g(u_0) = u_0$ we have that (10) becomes

$$\frac{\partial}{\partial t} e^{tL} u_0 = L e^{tL} u_0.$$

Remark: For stochastic systems this is called the backward Kolmogorov equation. The equation for the density is the Liouville equation (forward Kolmogorov equation).

Let $u_0 = (\hat{u}_0, \tilde{u}_0)$ where $\hat{u}_0$ is N-dimensional and $\tilde{u}_0$ is $M - N$ -dimensional. Define a projection operator $P : \mathcal{F}(u_0) \to \hat{\mathcal{F}}(\hat{u}_0)$. Also, define the operator $Q = I - P$.

$$\frac{\partial}{\partial t} e^{tL} u_{0k} = e^{tL} PLu_{0k} + e^{tL} QLu_{0k}$$

$$= e^{tL} PLu_{0k} + e^{tQL} QLu_{0k} + \int_0^t e^{(t-s)L} PLe^{sQL} QLu_{0k} ds \qquad (11)$$

for $k = 1, \ldots, N$.

We have used Dyson's formula (Duhamel's principle)

$$e^{tL} = e^{tQL} + \int_0^t e^{(t-s)L} PLe^{sQL} ds. \qquad (12)$$

If we write

$$e^{tQL} QLu_{0k} = w_k,$$

$w_k(u_0, t)$ satisfies the equation

$$\begin{cases} \frac{\partial}{\partial t} w_k(u_0, t) = QLw_k(u_0, t) \\ w_k(u_0, 0) = QLu_{0k} = R_k(u_0) - (PR_k)(\hat{u}_0). \end{cases} \tag{13}$$

The solution of (13) is at all times orthogonal to the range of P. We call it the orthogonal dynamics equation.

Remark: The difficulty with the orthogonal dynamics equation is that, in general, it cannot be written as a *closed* equation for $w_k(u_0, t)$. This means that its numerical solution is usually prohibitively expensive ("law of conservation of trouble").

Since the solutions of the orthogonal dynamics equation remain orthogonal to the range of P, we can project the Mori-Zwanzig equation (11) and find

$$\frac{\partial}{\partial t} P e^{tL} u_{0k} = P e^{tL} P L u_{0k} + P \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds. \quad (14)$$

Use (14) as the starting point of approximations for the evolution of the quantity $P e^{tL} u_{0k}$ for $k = 1, \ldots, N$ (note that equation (14) involves the orthogonal dynamics operator e^{tQL}).

Construct reduced models based on mathematical, physical and numerical observations.

These models come directly from the original equations and the terms appearing in them are not introduced by hand.

Since the solutions of the orthogonal dynamics equation remain orthogonal to the range of P, we can project the Mori-Zwanzig equation (11) and find

$$\frac{\partial}{\partial t} P e^{tL} u_{0k} = P e^{tL} P L u_{0k} + P \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds. \quad (14)$$

Use (14) as the starting point of approximations for the evolution of the quantity $Pe^{tL}u_{0k}$ for $k = 1, \ldots, N$ (note that equation (14) involves the orthogonal dynamics operator e^{tQL}).

Construct reduced models based on mathematical, physical and numerical observations.

These models come directly from the original equations and the terms appearing in them are not introduced by hand.

Fluctuation-dissipation theorems

Assume that one has access to the p.d.f. of the initial conditions, say $\rho(u_0)$.

1) Conditional expectation: For a function $f(u_0)$ we have

$$E[f(u_0)|\hat{u}_0] = \frac{\int f(u_0)\rho(u_0)d\tilde{u}_0}{\int \rho(u_0)d\tilde{u}_0}.$$

The conditional expectation is the best in an L_2 sense, meaning $E[|f - E[f|\hat{u}_0]|^2] \leq E[|f - h(\hat{u}_0)|^2]$ for all functions h.

2) Finite-rank projection: Denote the space of square-integrable functions of $\hat{u}_0$ as $\hat{L}_2$. Let $h_1(\hat{u}_0), h_2(\hat{u}_0), \ldots$ be an orthonormal set of basis functions of $\hat{L}_2$, i.e. $E[h_i h_j] = \delta_{ij}$ (w.r.t. the p.d.f. $\rho(u_0)$). Then,

$$(Pf)(\hat{u}_0) = \sum_{j=1}^{I} a_j h_j(\hat{u}_0),$$

where $a_j = E[fh_j]$, for $j = 1, \ldots, I$.

Remark: If we keep only the linear terms in the expansion, we get the so called “linear" projection, which is the most popular (implicit assumption of being near equilibrium).

Fluctuation-dissipation theorem of the first kind: Consider the case of only one resolved variable, say u_{01} and keep only the linear term in the projection, $Pf(u_0) = (f, u_{01})u_{01}$ where we assume $(u_{01}, u_{01}) = 1$. The MZ equation becomes

$$\frac{\partial}{\partial t} e^{tL} u_{01} = e^{tL} PLu_{01} + e^{tQL} QLu_{01} + \int_0^t e^{(t-s)L} PLe^{sQL} QLu_{01} ds,$$

or

$$\frac{\partial}{\partial t} e^{tL} u_{01} = (Lu_{01}, u_{01}) e^{tL} u_{01} + e^{tQL} QLu_{01} + \int_0^t (Le^{sQL} QLu_{01}, u_{01}) e^{(t-s)L} u_{01} ds. \quad (15)$$

We take the inner product of (15) with u_{01} and find

$$\begin{aligned}\frac{\partial}{\partial t}(e^{tL}u_{01},u_{01}) &= (Lu_{01},u_{01})(e^{tL}u_{01},u_{01}) \\ &+ (e^{tQL}QLu_{01},u_{01}) + \int_0^t (Le^{sQL}QLu_{01},u_{01})e^{(t-s)L}u_{01}\,ds \\ &= (Lu_{01},u_{01})(e^{tL}u_{01},u_{01}) \\ &+ \int_0^t (Le^{sQL}QLu_{01},u_{01})(e^{(t-s)L}u_{01},u_{01})ds, \quad (16)\end{aligned}$$

because $Pe^{tQL}QLu_{01} = (e^{tQL}QLu_{01},u_{01})u_{01} = 0$ and hence $(e^{tQL}QLu_{01},u_{01}) = 0$.

Remark: Equation (16) describes the evolution of the autocorrelation $(e^{tL}u_{01},u_{01})$.

Multiply equation (16) with u_{01} and recall that $Pe^{tL}u_{01} = (e^{tL}u_{01},u_{01})u_{01}$.

We find

$$\frac{\partial}{\partial t} P e^{tL} u_{01} = (L u_{01}, u_{01}) P e^{tL} u_{01} + \int_0^t (L e^{sQL} Q L u_{01}, u_{01}) P e^{(t-s)L} u_{01}. \tag{17}$$

$$\frac{\partial}{\partial t} (e^{tL} u_{01}, u_{01}) = (L u_{01}, u_{01})(e^{tL} u_{01}, u_{01}) + \int_0^t (L e^{sQL} Q L u_{01}, u_{01})(e^{(t-s)L} u_{01}, u_{01}) ds. \tag{18}$$

Remark: Equation (17) describes the evolution of $P e^{tL} u_{01}$ which is a non-equilibrium quantity. Equation (18) describes the evolution of $(e^{tL} u_{01}, u_{01})$ which is an equilibrium quantity (in fact an autocorrelation). But these are the same equations!!

This is the *fluctuation-dissipation theorem of the first kind* also known as *Onsager's principle*.

Fluctuation-dissipation theorem of the second kind:
Assume that P is the finite-rank projection. Since the quantity $e^{tQL}QLu_{01}$ starts and stays in the space orthogonal to the range of P, we have $e^{tQL}QLu_{01} = Qe^{tQL}QLu_{01}$. For the memory term kernel we find

$$PLe^{sQL}QLu_{0k} = PLQe^{sQL}QLu_{0k}$$

$$= \sum_{j=1}^{l} (LQe^{sQL}QLu_{0k}, h_j(\hat{u}_0))h_j(\hat{u}_0)$$

For Hamiltonian systems, if one uses the Boltzmann distribution to define the inner product then the operator L is skew-symmetric. This holds more generally.

Proposition:If the density used to define the inner product is invariant and the projection used is the finite-rank one, then the operator L is skew-symmetric.

If the assumptions of the theorem hold then

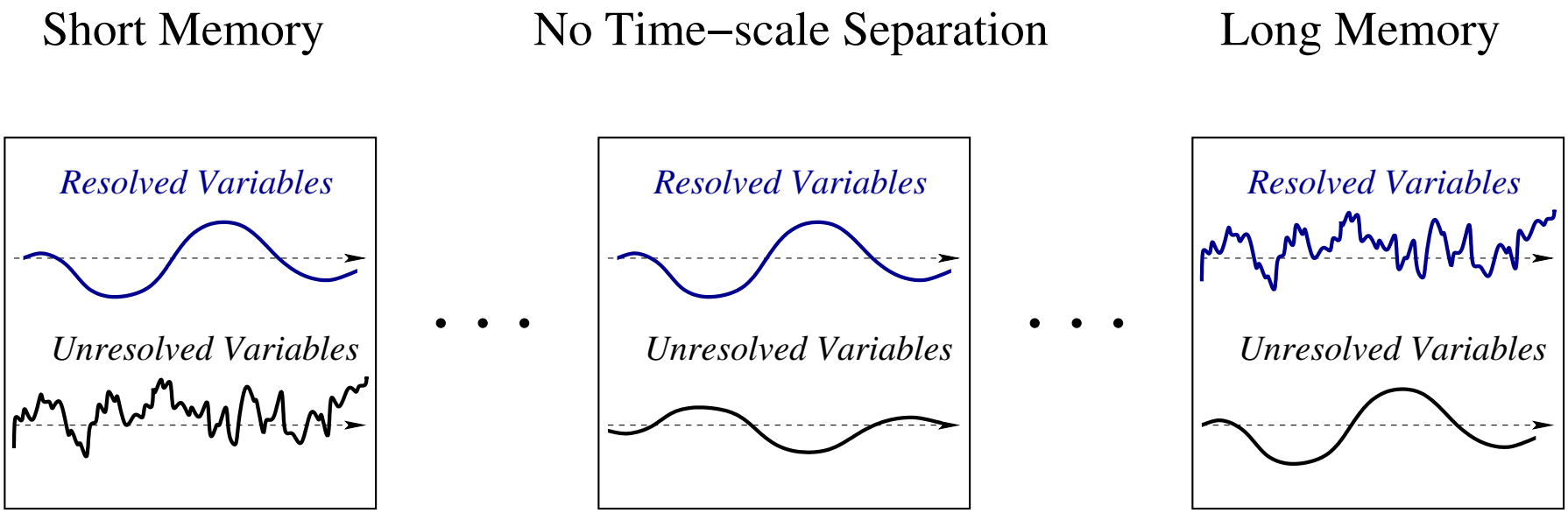
$$PLe^{sQL}QLu_{01} = -\sum_{j=1}^{l}(e^{sQL}QLu_{0k}, QLh_j(\hat{u}_0))h_j(\hat{u}_0)$$

Remark: All the memory kernels become correlations of different orders. In particular, for the linear function $h(\hat{u}_0) = u_{0k}$ we have the noise autocorrelation $(e^{sQL}QLu_{0k}, QLu_{0k})$.

The minus sign means that in this case, the memory term is dissipative in nature. Thus, the noise term i.e., the fluctuations are related to the memory term i.e., the dissipation. This is the *fluctuation-dissipation theorem of the second kind*.

It is very popular in statistical physics and molecular dynamics.

Time-scale classification



The short-time and short-memory approximations

We rewrite Dyson's formula as

$$e^{tQL} = e^{tL} - \int_0^t e^{(t-s)L} PLe^{sQL} ds$$

Make the following approximation

$$e^{tQL} \cong e^{tL}$$

In other words, we replace the flow in the orthogonal complement of $\mathcal{F}$ with the flow induced by the full system operator L.

Remark: We expect such an approximation to be valid *only* for short times, unless there is a special structure of the full system.

$$\int_0^t e^{(t-s)L} PLe^{sQL} QLu_{0k} ds = \int_0^t e^{(t-s)L} PL(P+Q)e^{sQL} QLu_{0k} ds$$
$$= \int_0^t e^{(t-s)L} PLQe^{sQL} QLu_{0k} ds, \quad (19)$$

since $Pe^{sQL} QLu_{0k} = 0$. Adding and subtracting equal quantities, we find

$$PLQe^{sQL} QLu_{0k} = PLQe^{sL} QLu_{0k} + PLQ(e^{sQL} - e^{sL})QLu_{0k} \quad (20)$$

Expanding in Taylor series the difference we have

$$e^{sQL} - e^{sL} = I + sQL + \cdots - I - sL - \cdots = -sPL + O(s^2), \quad (21)$$

and thus

$$Q(e^{sQL} - e^{sL}) = O(s^2), \quad (22)$$

using $QP = 0$. Substituting (22) in (20) we find

Consider the case where P is the finite-rank projection so

$$PLQe^{sQL}QLu_{0k} = \sum_{j=1}^{l}(LQe^{sQL}QLu_{0k}, h_j(\hat{u}_0))h_j(\hat{u}_0), \qquad (24)$$

and for the approximation

$$PLQe^{sL}QLu_{0k} = \sum_{j=1}^{l}(LQe^{sL}QLu_{0k}, h_j(\hat{u}_0))h_j(\hat{u}_0). \qquad (25)$$

If we truncate the memory after t_0 units of time then

$$\begin{aligned}\int_0^t e^{(t-s)L}PLe^{sQL}QLu_{0k}ds &\approx \int_0^{t_0} e^{(t-s)L}PLQe^{sQL}QLu_{0k}ds \\ &= \int_0^{t_0} e^{(t-s)L}PLQe^{sL}QLu_{0k}ds + \int_0^{t_0} O(s^2)ds \\ &= \int_0^{t_0} e^{(t-s)L}PLQe^{sL}QLu_{0k}ds + O(t_0^3).\end{aligned}$$

Remark: The short-time approximation is valid for large times if t_0 is small. On the other hand, if t_0 is large, then the error is $O(t^3)$ and the approximation is only valid for short times.

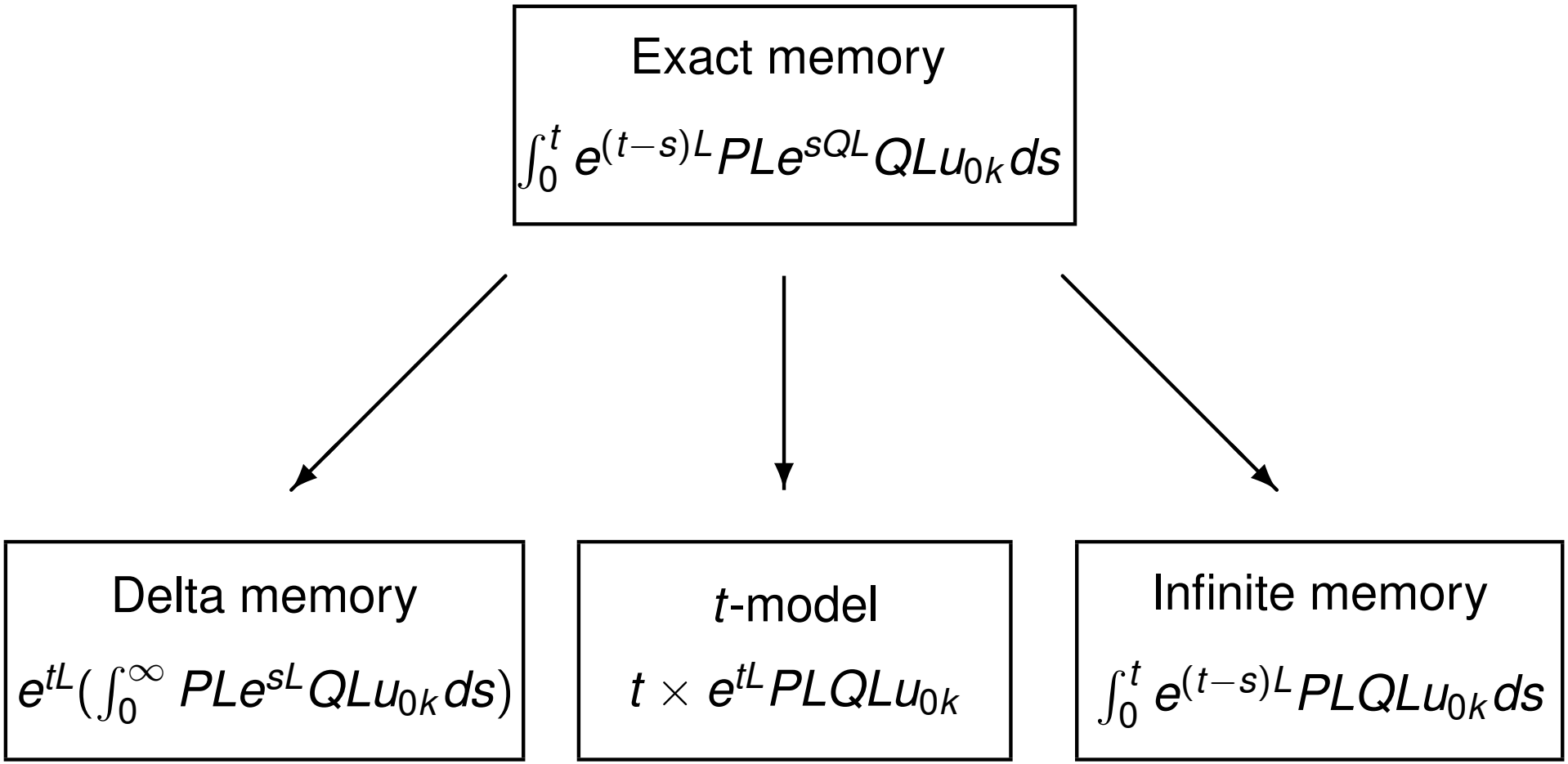
Remark: The short-memory approximation contains the delta-function approximation used in statistical physics as a special case.

The short-memory approximation equations are

$$\frac{\partial}{\partial t} e^{tL} u_{0k} = e^{tL} PLu_{0k} + e^{tL} QLu_{0k} + \int_0^{t_0} e^{(t-s)L} PLe^{sL} QLu_{0k} ds$$

for $k = 1, \ldots, N$.

Simplest possible approximations



Absence of time-scale separation

The short-memory case while easier to deal with is not the prevalent one in real-world applications. Of course, one can think of developing methods which identify “slow" resolved and “’fast" unresolved variables and construct a reduced model for the slow ones.

This is easier said than done because the “slow" variables should also have some physical significance. This is not obvious if the “slow" variables turn out to be highly nonlinear combinations of the underlying variables.

For intermediate memory length, the necessary memory kernels can be found through a Volterra integral equation formulation starting from Dyson’s formula. One computes only certain correlations of the orthogonal dynamics (see the work of Chorin, Hald, Kupferman, Darve and Karniadakis).

However, this may not be enough either. In particular, the resolved variables may not only evolve on timescales which are comparable with those of the unresolved variables but the unresolved variables could be too many to even run the full system once.

One way of addressing this situation is to accept the absence of time-scale separation between the original variables and develop reduced models based on a different classification.

To proceed in this direction we need to look at the classification of systems according to size (cardinality, number of active length and/or timescales).

This classification can help us to identify new “small" quantities for which one can formulate (singular) perturbation expansions.

System size classification

$|S1|$: Size of original system
$|S2|$: Size of full system (available computational power)
$|S3|$: Size of reduced system

1. $|S2| >> |S1|$: Possible to run multiple simulations of the original system. E.g. Linearized flows, certain chemical kinetics systems.

2. $|S2| \approx |S1|$: Possible to run a single simulation of the original system. E.g. Molecular dynamics.

3. $|S2| << |S1|$: Not possible to run even a single simulation of the original system. E.g. Atmosphere/ocean dynamics, fluid/structure interaction, singular PDEs.

System size classification

$|S1|$: Size of original system
$|S2|$: Size of full system (available computational power)
$|S3|$: Size of reduced system

1. $|S2| >> |S1|$**:** Possible to run multiple simulations of the original system. E.g. Linearized flows, certain chemical kinetics systems.

2. $|S2| \approx |S1|$**:** Possible to run a single simulation of the original system. E.g. Molecular dynamics.

3. $|S2| << |S1|$**:** Not possible to run even a single simulation of the original system. E.g. Atmosphere/ocean dynamics, fluid/structure interaction, singular PDEs.

System size classification

$|S1|$: Size of original system
$|S2|$: Size of full system (available computational power)
$|S3|$: Size of reduced system

1. $|S2| >> |S1|$: Possible to run multiple simulations of the original system. E.g. Linearized flows, certain chemical kinetics systems.

2. $|S2| \approx |S1|$: Possible to run a single simulation of the original system. E.g. Molecular dynamics.

3. $|S2| << |S1|$: Not possible to run even a single simulation of the original system. E.g. Atmosphere/ocean dynamics, fluid/structure interaction, singular PDEs.

Simplest model with absence of time-scale separation

The memory term $\int_0^t e^{(t-s)L} PLe^{sQL} QLu_{0k} ds$ involves two evolution operators, the full dynamics operator e^{tL} and the orthogonal dynamics operator e^{tQL}.

The full dynamics operator evolves on a time scale τ_f and the orthogonal dynamics operator evolves on the time-scale τ_o. There are three major cases: i) $\tau_f \gg \tau_o$, ii) $\tau_f \sim \tau_o$, and iii) $\tau_f \ll \tau_o$.

If we assume that both $e^{(t-s)L}$ and e^{sQL} are analytic, we can expand the expression $e^{(t-s)L} PLe^{sQL}$ in Taylor series around $s = 0$.

If we keep only the zero order term in both expansions we get $\int_0^t e^{(t-s)L} PLe^{sQL} QLu_{0k} ds = te^{tL} PLQLu_{0k} + O(t^2)$ which is called the t-model.

Remark: The t-model contains no adjustable parameters (good and bad).

1) Is the t-model stable, convergent?

2) Can it be used to track singularities?

3) What about the higher order terms? —-> A sea of instabilities

4) What can be done?

1D Burgers equation

$$v_t + PB(v, v) = -tP[B(v, \Gamma) + B(\Gamma, v)]$$

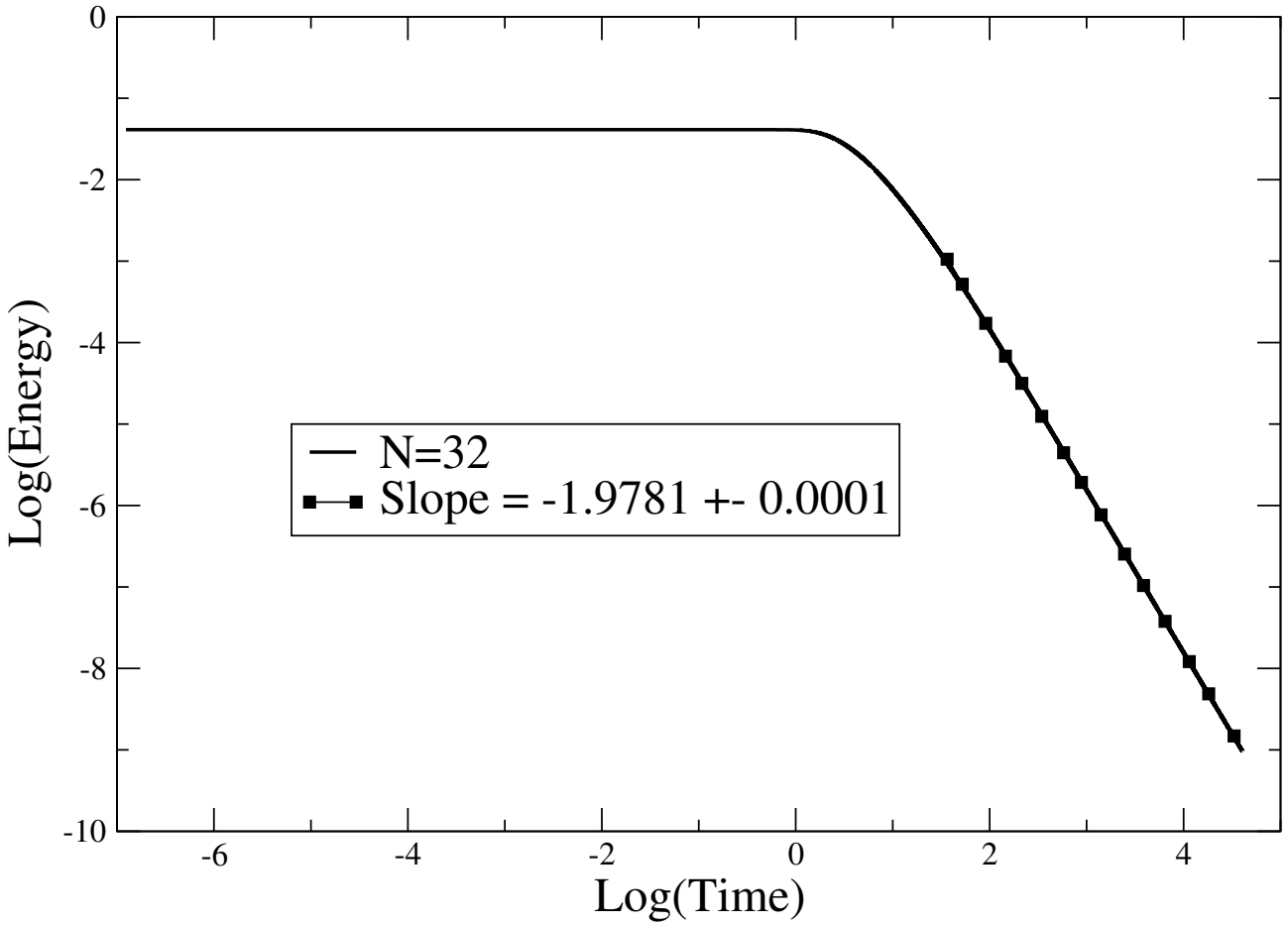
where $B(g, h) = \frac{1}{2}(gh)_x$ and $\Gamma = -(I - P)B(v, v)$.

1D focusing nonlinear Schrödinger equation

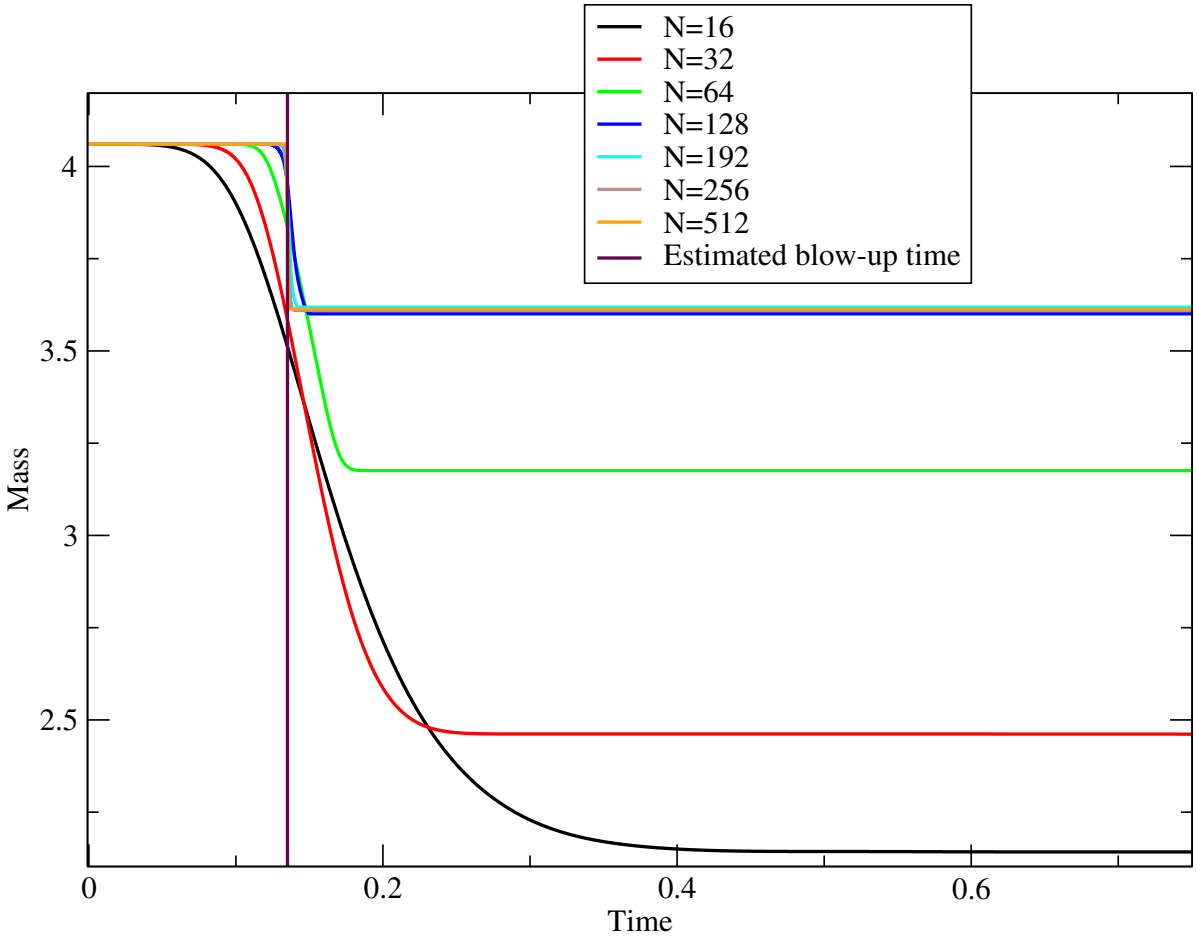
$$v_t - i\Delta v + iPB[v, v, v, v, v] = i3tPB[\Gamma, v, v, v, v] + i2tPB[v, \Gamma, v, v, v].$$

where $B[z_1, z_2, z_3, z_4, z_5] = z_1 z_2^* z_3 z_4^* z_5$ and
$\Gamma(x, t) = i(I - P)B[v, v, v, v, v]$.

Similarly, construct t-model for Euler and Navier-Stokes equations.



Energy evolution of the t-model with $N = 32$ modes for the inviscid Burgers equation with $u_0(x) = \sin x$.



Mass evolution of the *t*-model for the 1D critical Schrödinger equation. The vertical line denotes the numerically estimated blow-up instant calculated with a mesh refinement algorithm.

Higher order models

Through Dyson's formula and the linearity of e^{tL} the memory term can be written as

$$\int_0^t e^{(t-s)L} PLe^{sQL} QLu_{0k}\, ds = e^{tL}\left(QLu_{0k} - e^{-tL}e^{tQL}QLu_{0k}\right)$$

Now we will employ the identity $I = P + Q$ and the Baker-Campbell-Hausdorff (BCH) series for $e^{-tL}e^{tQL}$. The BCH formula reads $e^{-tL}e^{tQL} = e^{C(t,u_0)}$ where

$$C(t,u_0) = -tL + tQL + \frac{1}{2}[-tL, tQL]$$
$$+\frac{1}{12}\Big([-tL,[-tL,tQL]] + [tQL,[tQL,-tL]]\Big) + \dots$$
$$= -tPL - \frac{1}{2}[tPL, tQL]$$
$$+\frac{1}{12}\Big([-tL,-[tPL,tQL]] + [tQL,-[tQL,tPL]]\Big) + \dots$$

Remark: All the higher terms involve the commutator $[-tL, tQL] = -tLtQL - tQL(-tL)$. Also, the last equality comes from noting that $[-tL, tQL] = [tL, tPL] = [tQL, tPL] = -[tPL, tQL]$.

We find that

$$\int_0^t e^{(t-s)L} PLe^{sQL} QLu_{0k} ds = e^{tL}\left(QLu_{0k} - e^{C(t,u_0)} QLu_{0k}\right) \quad (26)$$

Remark: Note that the first term in the BCH series is the operator $-tPL$. It is very helpful computationally if we can keep this term and discard the higher order ones because it involves only the projected dynamics. We want to examine when is the approximation $C(t, u_0) \approx -tPL$ acceptable.

From the BCH series we have

$$e^{-tL}e^{tQL} - e^{-tPL} = -\frac{1}{2}[tPL, tQL] + O(t^3). \quad (27)$$

Depending on the initial conditions, $[PL, QL]$ may be small and thus allow the simplification of the memory term expression.

If we assume that $[PL, QL] \approx 0$ and thus $C(t, u_0) \approx -tPL$, then from (26) we get

$$\int_0^t e^{(t-s)L} PL e^{sQL} QL u_{0k} ds \approx e^{tL} \left(QL u_{0k} - e^{-tPL} QL u_{0k} \right)$$

Expansion of the operator e^{-tPL} in Taylor series around $t = 0$ gives

$$P \int_0^t e^{(t-s)L} PL e^{sQL} QL u_{0k} ds \approx \tag{28}$$

$$\sum_{j=1}^{\infty} (-1)^{j+1} \frac{t^j}{j!} P e^{tL} (PL)^j QL u_{0k}.$$

Remark: This approximation turns out to be unstable but it also suggests the next step.

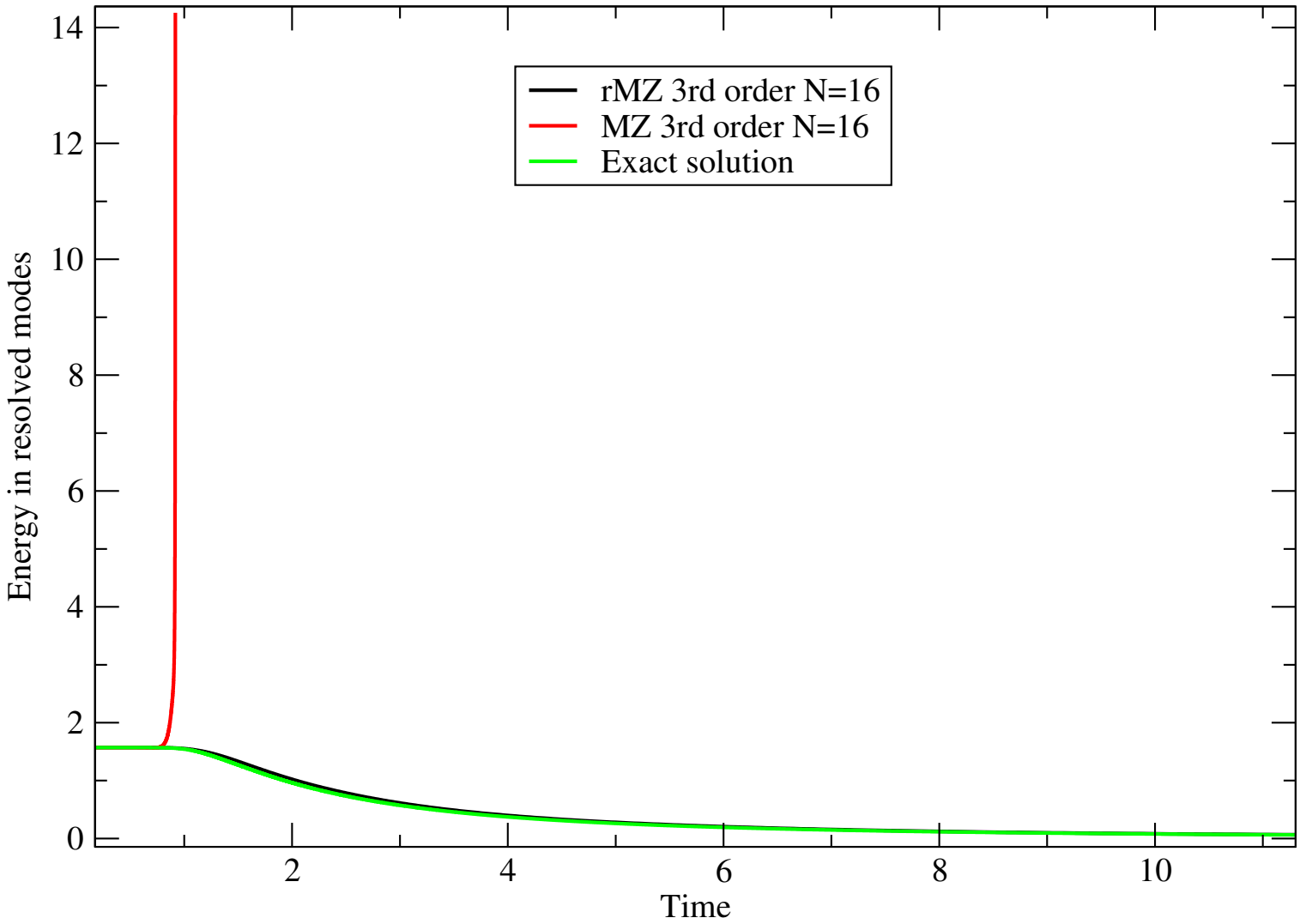


Figure : Evolution of energy content of resolved modes for inviscid 1D Burgers equation

Scale dependence and renormalization

It may be possible to "renormalize" the expansion.

What does this mean?

1) Embed the MZ reduced models in a larger class of reduced models which share the same functional form as the MZ reduced models but have different coefficients in front of the memory terms.

2) One can estimate these coefficients on the fly while the full system is still well resolved.

Remark: Because we are interested in dynamic phenomena this is time-dependent renormalization (extra complication).

The renormalized expansion

$$P\int_0^t e^{(t-s)L}PLe^{sQL}QLu_{0k}\,ds \approx \sum_{j=1}^{\infty}\alpha_j(-1)^{j+1}\frac{t^j}{j!}Pe^{tL}(PL)^jQLu_{0k}.$$

The renormalized coefficients α_j are dimensionless by construction.

Estimate the coefficients by requiring that the reduced model reproduces certain important features of the full system.

Remark: The reduced model should capture accurately the rate of transfer of activity (e.g. mass, energy) from resolved to unresolved scales.

Scaling laws and renormalization for singularities (rMZ)

Main idea: The renormalized coefficients have a scaling law dependence on the smoothness of the initial condition

Remark: By *smoothness of initial condition* we mean the ratio of the largest Fourier mode present in the initial condition to the largest Fourier mode that is resolved by the reduced model

Remark: 1) There are dependencies between the renormalized coefficients of different order. 2) Order by order perturbative renormalization is not enough

Remark: Example, for 1D Burgers, 3rd order rMZ with $a_1 = \alpha\left(\frac{1}{N/2-\beta_1}\right)$ and $a_2 = a_1\left(\frac{1}{N/2-\beta_2}\right)$ and $a_3 = a_2\left(\frac{1}{N/2-\beta_3}\right)$ where $\alpha = 1.532, \beta_1 = 0.452, \beta_2 = -0.661$ and $\beta_3 = 0.728$ and where N is the total number of Fourier modes.

“Proper” coarse-grained variables

For each problem it is important to concentrate on the relevant degrees of freedom (Weinberg, 1983)

Remark: We would like to find variables that facilitate the construction of a reduced model

Main idea: Choose variables for which the initial condition is smooth. Then apply the previous renormalization arguments (perturbative renormalization)

Remark: Such variables can be found by basis adaptation, active subspaces, compressed sensing, empirical orthogonal eigenfunction expansion, principal component analysis etc.

Remark: The renormalization of the coefficients has connections with *incomplete similarity*.

Remark: Non-perturbative renormalization (resolved variable function space expansion).

Some references

- Chorin A.J., Hald O.H. and Kupferman R., Optimal prediction with memory, Physica D 166 (2002) pp. 239-257.
- Darve E., Solomon J. and Kia A., Computing generalized Langevin equations and generalized Fokker-Planck equations, PNAS 106 (27) (2009) pp. 10884-10889.
- Li Z., Bian X., Caswell B. and Karniadakis G.E., Construction of dissipative particle dynamics models for complex fluids via the Mori-Zwanzig formulation, Soft Matter 10(43) (2014) pp. 8659-72.
- P. S., Numerical computation of solutions of the critical nonlinear Schrödinger equation after the singularity, Multiscale Modeling and Simulation 10 (2012), pp. 48-60.
- P.S., Renormalized Mori-Zwanzig reduced models for systems without scale separation, Proceedings of the Royal Society A Vol. 471 (2015) No. 2176.