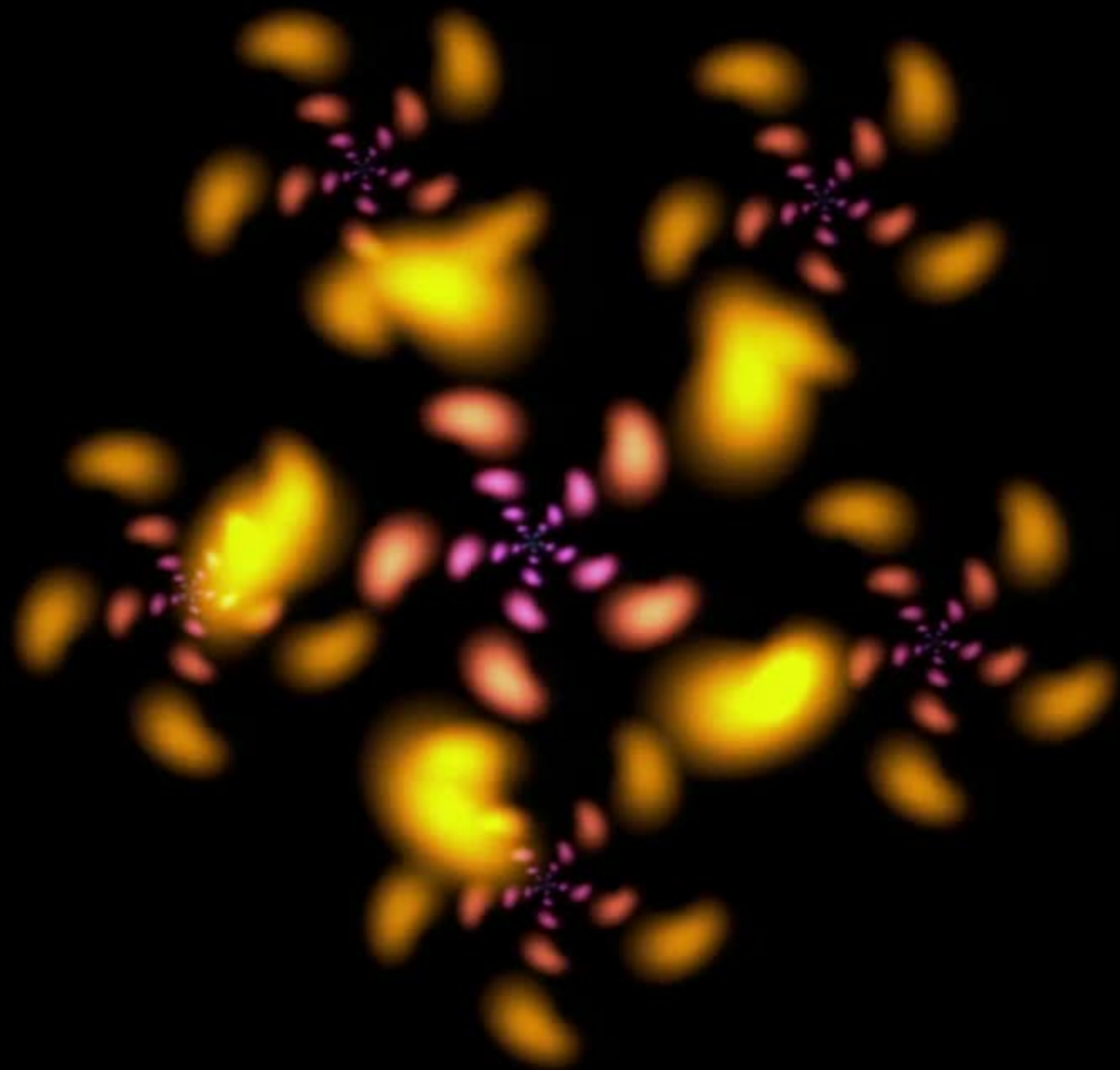


# Reduced order models for uncertainty quantification of time-dependent problems

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Pacific Northwest National Laboratory





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# Uncertainty in time-dependent problems

In many time-dependent problems of practical interest, parameters and/or initial/boundary conditions can be uncertain.

One way to address the problem of how this uncertainty impacts the solution is to expand the solution using polynomial chaos expansions and obtain a system of differential equations for the evolution of the expansion coefficients.

**Main idea:** Construct reduced models for a *subset* of the polynomial chaos expansion coefficients that are needed for a full description of the uncertainty.

We will use the Mori-Zwanzig formalism to construct such reduced models.

**Remark:** *Accurate* reduced models require memory *even* for simple systems.

**Remark:** The construction of *accurate* reduced models can be very costly *even* for simple systems.

# The Mori-Zwanzig formalism

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

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

$$\frac{du(t)}{dt} = R(u(t)) \quad (1)$$

with initial condition  $u(0) = u_0$ .

Transform into a system of linear partial differential equations

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

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



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  $P : \mathcal{F}(u_0) \rightarrow \hat{\mathcal{F}}(\hat{u}_0)$ . Also, define the operator  $Q = I - P$ .

$$\frac{\partial}{\partial t} e^{tL} u_{0k} = e^{tL} P L u_{0k} + e^{tQL} Q L u_{0k} + \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds \quad (2)$$

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

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

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Use (4) as the starting point of approximations for the evolution of the quantity  $P e^{tL} u_{0k}$  for  $k = 1, \dots, N$  (note that the equation (4) 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.**



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# Scalar linear differential equation

Consider

$$\frac{du}{dt} = -\kappa u, \quad (5)$$

where  $\kappa \sim U[0, 1]$ . Let  $u \approx \sum_{r=0}^M u_r L_r(w)$ , where  $w \sim U[-1, 1]$  and  $\{L_r\}$  are the Legendre polynomials. We obtain

$$\frac{du_r}{dt} = - \sum_{i=0}^1 \sum_{j=0}^M k_{ijr} u_j, \quad r = 0, \dots, M, \quad (6)$$

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**Remark:** To compute the memory term in *closed form* we need to introduce a finite-rank projection (in addition to  $P$ ). We use

$$(P' \varphi_j)(\hat{u}, t) \approx \sum_{\nu} (\varphi_j(u, t), h^{\nu}(\hat{u})) h^{\nu}(\hat{u}),$$

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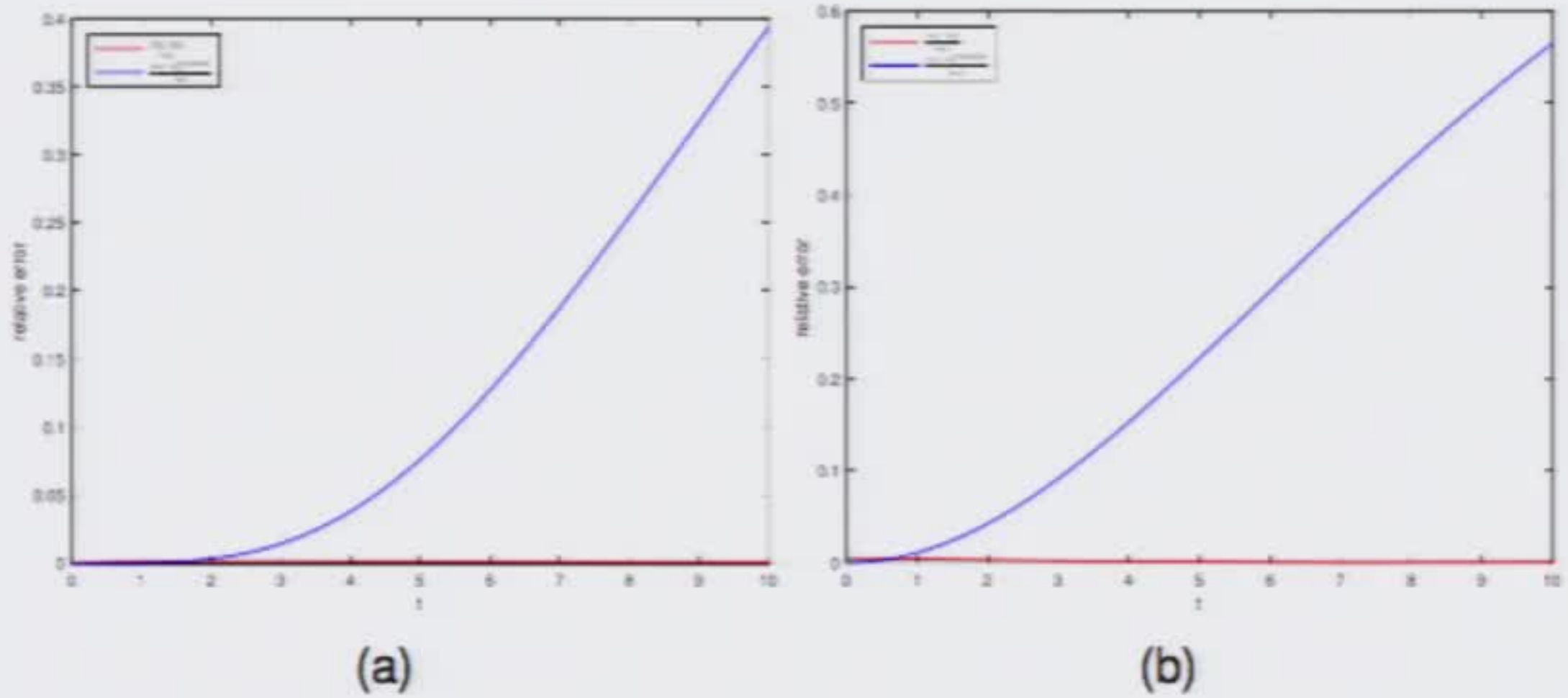
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where  $h^{\nu}$  are Hermite polynomials.



**Figure:** Comparison of the relative error for the models with and without memory for the linear equation with uncertain coefficient.

**Remark:** Memory is very important for accurate prediction even for moderate times.



# Periodically forced nonlinearly damped particle

Consider

$$\frac{du}{dt} = u - u^3 + f(t, w), \quad (7)$$

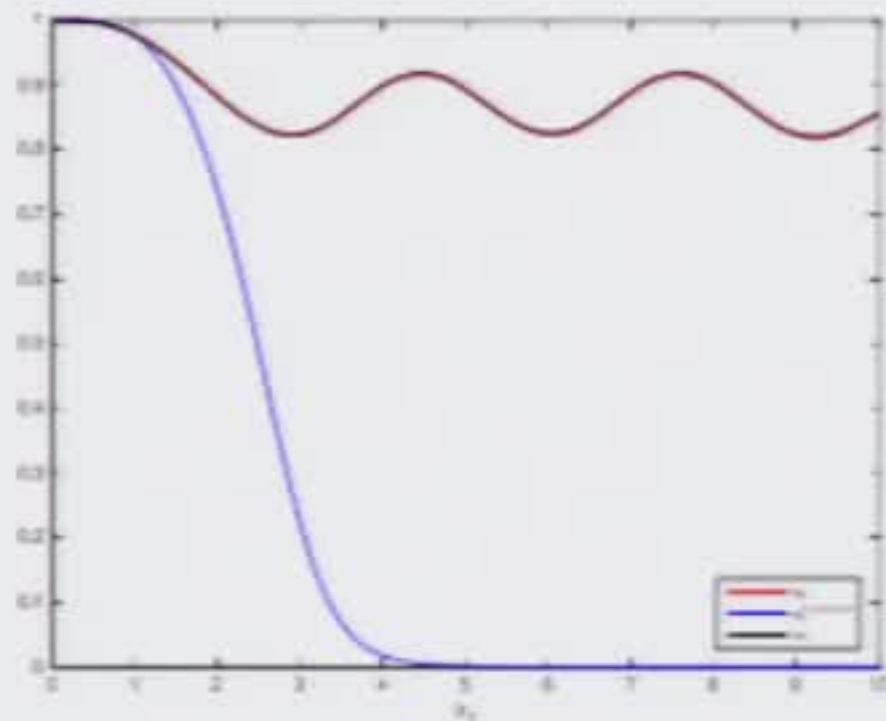
where  $f = w \sin t$  and  $w \sim U(-1, 1)$ . Let  $u \approx \sum_{i=0}^M u_i L_i(w)$ , where  $w \sim U[-1, 1]$  and  $\{L_i\}$  are the Legendre polynomials. We obtain

$$\frac{du_i}{dt} = u_i - \sum_{j,k,m=0}^{P_f} u_j u_k u_m e_{jkm i} + f_i, \quad i = 0, \dots, M, \quad (8)$$

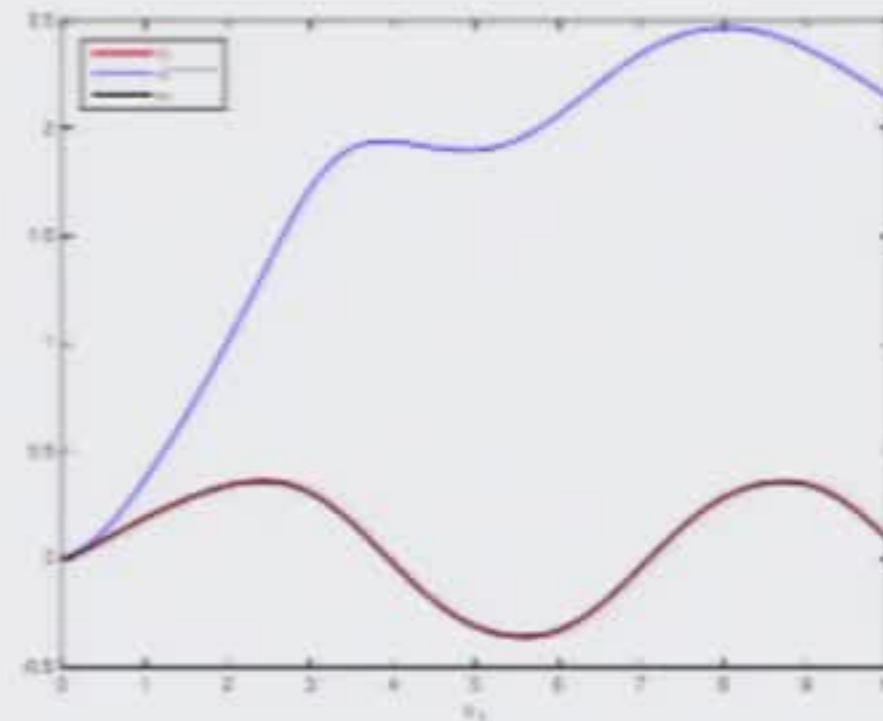
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**Remark:** To compute the memory term in *closed form* we need to introduce a finite-rank projection (in addition to  $P$ ). We use Hermite polynomials as before.



(a)

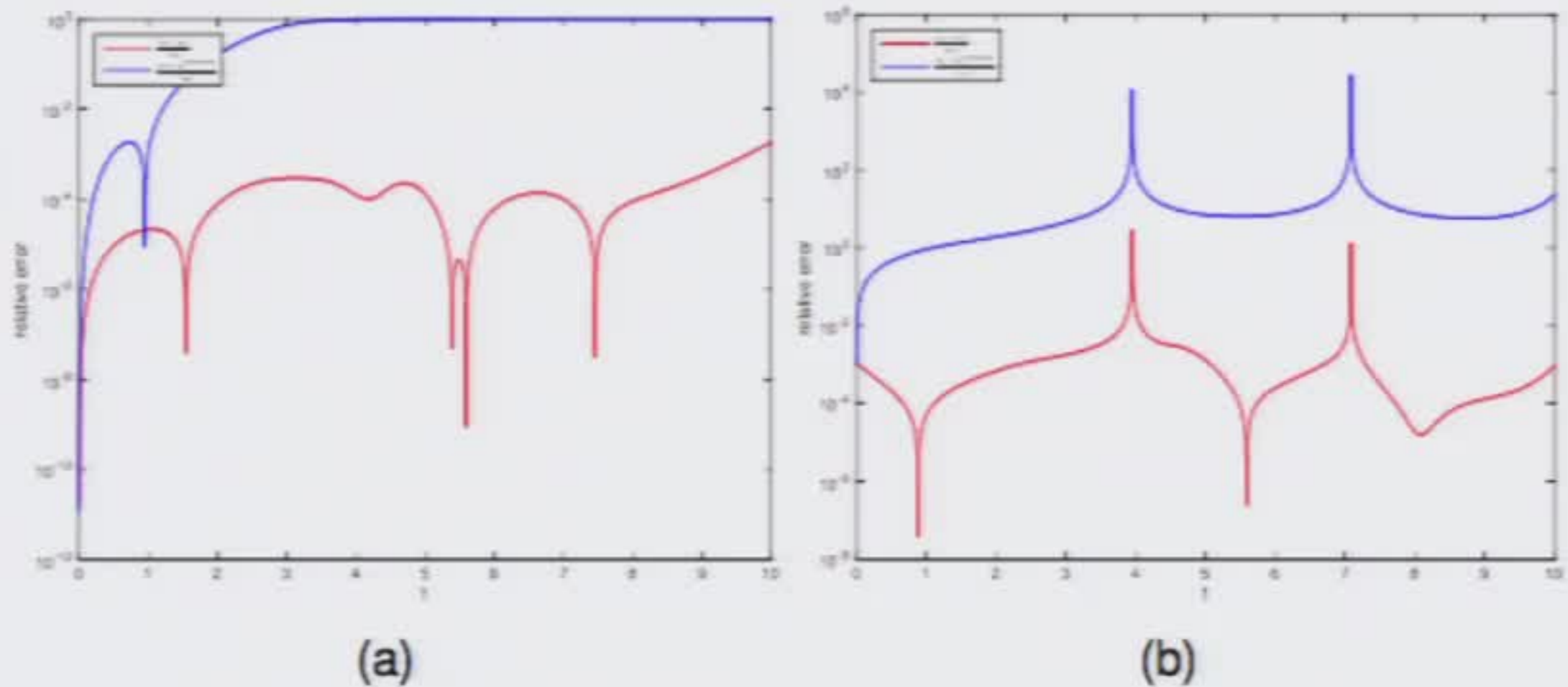


(b)

**Figure:** Comparison of the solution without memory, with memory and exact solution for the periodically forced damped particle equation.

**Remark:** We construct a reduced model with  $\Lambda = 1$  and  $M = 6$ . The model with memory uses 10 basis functions (highest order 3) for the memory term integrand. The integrands for the memory term can be computed by solving Volterra equations.





**Figure:** Comparison of the relative error (logarithmic scale) for the models with and without memory for the periodically forced damped particle equation.

**Remark:** Memory is very important for accurate prediction even for short times.

# Application to the 1D Burgers equation

Consider the Burgers equation

$$u_t + uu_x = \nu u_{xx}. \quad (9)$$

We assume periodic BCs and  $u(0, x) = u_0(x)$ .

We can have e.g. uncertain viscosity coefficient and/or uncertain initial conditions.

For a simple case with  $\nu = 0.03$  one needs about 100 Fourier modes to resolve the solution. If e.g.  $u_0(x, \xi) = (1 + \xi) \sin x$  where  $\xi \sim U[-1, 1]$ , we need the first 7 Legendre polynomials to fully resolve the uncertainty in the solution.

**Remark:** If we resolve 2 of the 7 expansion coefficients, then for the memory term we would need to have a basis in  $100 \times 2$  dimensions. It is prohibitively expensive to use with high orders.



**Remark:** If we have some prior information about the system then we may be able to reduce the number of arguments of the basis functions. Otherwise, we need to compute the term  $P \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds$  **without** relying on a finite-rank projection.

**Main idea:** Construct a hierarchy of equations for the evolution of the memory term and its derivatives.

Let  $w_{0k}(t) = P \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds$ . We find

$$\frac{dw_{0k}}{dt} = P e^{tL} P L Q L u_{0k} - P e^{(t-t_0)L} P L e^{t_0QL} Q L u_{0k} + w_{1k}(t)$$

where

$$w_{1k}(t) = P \int_{t-t_0}^t e^{sL} P L e^{(t-s)QL} Q L Q L u_{0k} ds$$

and we have assumed that the memory extends only  $t_0$  units back.

Also

$$\frac{dw_{1k}}{dt} = Pe^{tL} PLQLQLU_{0k} - Pe^{(t-t_0)L} PLe^{t_0 QL} QLQLU_{0k} + w_{2k}(t),$$

where

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This hierarchy continues

$$\frac{dw_{(n-1)k}}{dt} = Pe^{tL} PL(QL)^{n-1} QLU_{0k} - Pe^{(t-t_0)L} PLe^{t_0 QL} (QL)^{n-1} QLU_{0k} + w_{nk}(t)$$

where

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Of course, this is the *closure* problem which we can address by assuming that  $w_{nk}(t) = 0$ .



In addition to the closure, we have to estimate the terms  $Pe^{(t-t_0)L}PLe^{t_0QL}QLu_{0k}, \dots, Pe^{(t-t_0)L}PLe^{t_0QL}(QL)^{n-1}QLu_{0k}$ . This can be achieved by using a discretized version e.g. trapezoidal rule for  $w_{0k}(t), \dots, w_{(n-1)k}(t)$  and solving for the unknown terms.

**Remark:** The expansion above amounts to an expansion of the evolution operator for the *orthogonal dynamics* equation. There are alternative expansions which involve the *full dynamics* operator.

**Remark:** There is an unknown parameter, the length  $t_0$  of the memory. One can compute estimate  $t_0$  using a construction akin to renormalization. The estimate of  $t_0$  is determined through an optimization problem.

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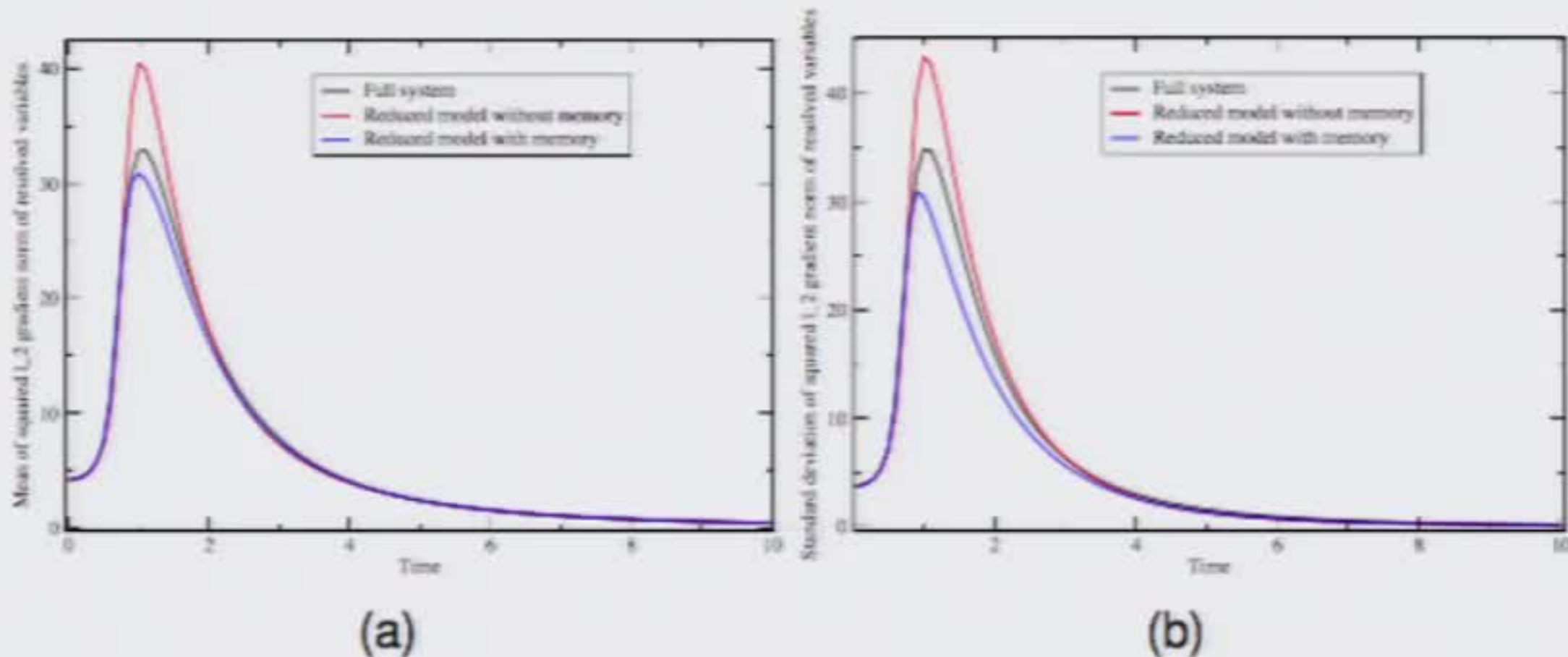


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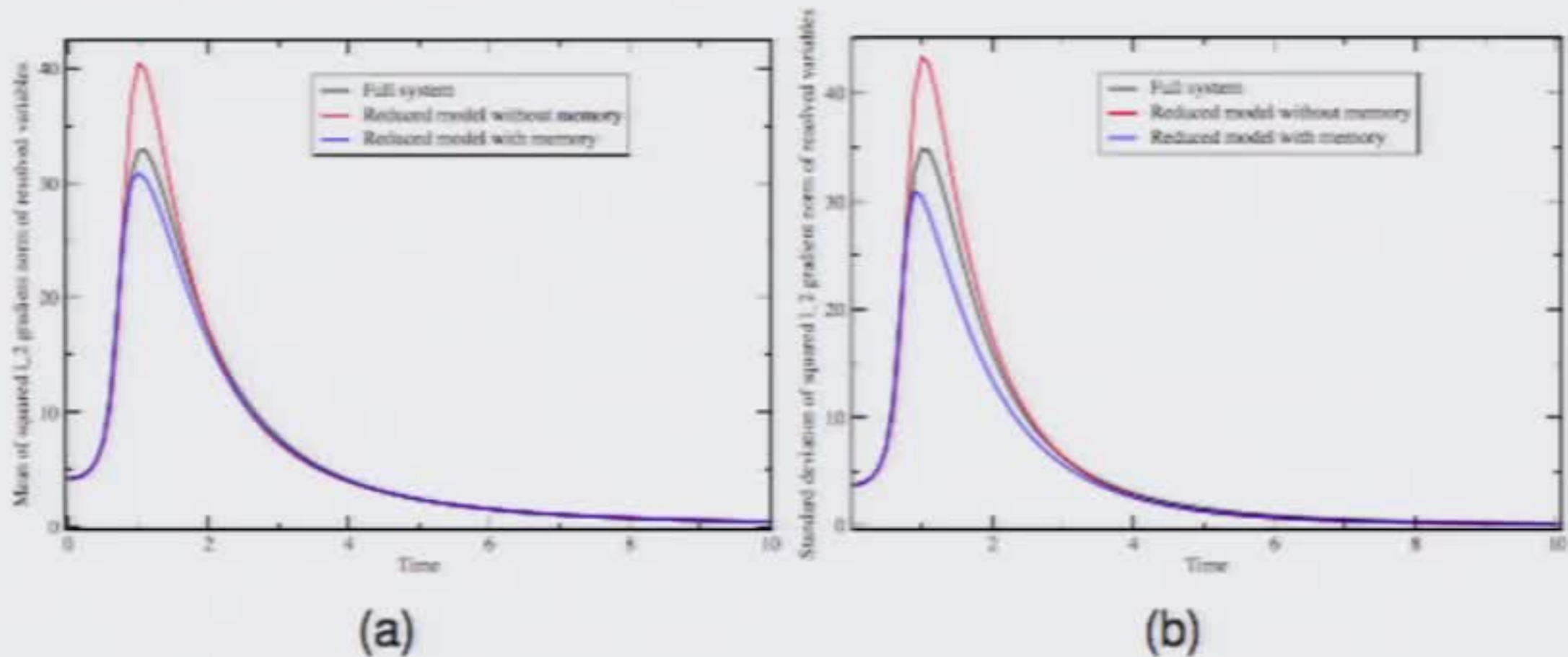
**Figure:** Evolution of the mean and the standard deviation of the gradient of the solution using only the first two Legendre polynomials.

**Conclusion:** The construction of reduced models for UQ can be necessary and costly. It must account for memory effects.



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where

$$w_{1k}(t) = P \int_{t-t_0}^t e^{sL} P L e^{(t-s)QL} Q L Q L u_{0k} ds$$

and we have assumed that the memory extends only  $t_0$  units back.

# Application to the 1D Burgers equation

Consider the Burgers equation

$$u_t + uu_x = \nu u_{xx}. \quad (9)$$

We assume periodic BCs and  $u(0, x) = u_0(x)$ .

We can have e.g. uncertain viscosity coefficient and/or uncertain initial conditions.

For a simple case with  $\nu = 0.03$  one needs about 100 Fourier modes to resolve the solution. If e.g.  $u_0(x, \xi) = (1 + \xi) \sin x$  where  $\xi \sim U[-1, 1]$ , we need the first 7 Legendre polynomials to fully resolve the uncertainty in the solution.

**Remark:** If we resolve 2 of the 7 expansion coefficients, then for the memory term term we would need to have a basis in  $100 \times 2$  dimensions. It is prohibitively expensive to use with high orders.



**Remark:** If we have some prior information about the system then we may be able to reduce the number of arguments of the basis functions. Otherwise, we need to compute the term  $P \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds$  **without** relying on a finite-rank projection.

**Main idea:** Construct a hierarchy of equations for the evolution of the memory term and its derivatives.

Let  $w_{0k}(t) = P \int_0^t e^{(t-s)L} P L e^{sQL} Q L u_{0k} ds$ . We find

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**Remark:** If we resolve 2 of the 7 expansion coefficients, then for the memory term we would need to have a basis in  $100 \times 2$  dimensions. It is prohibitively expensive to use with high orders.



# Periodically forced nonlinearly damped particle

Consider

$$\frac{du}{dt} = u - u^3 + f(t, w), \quad (7)$$

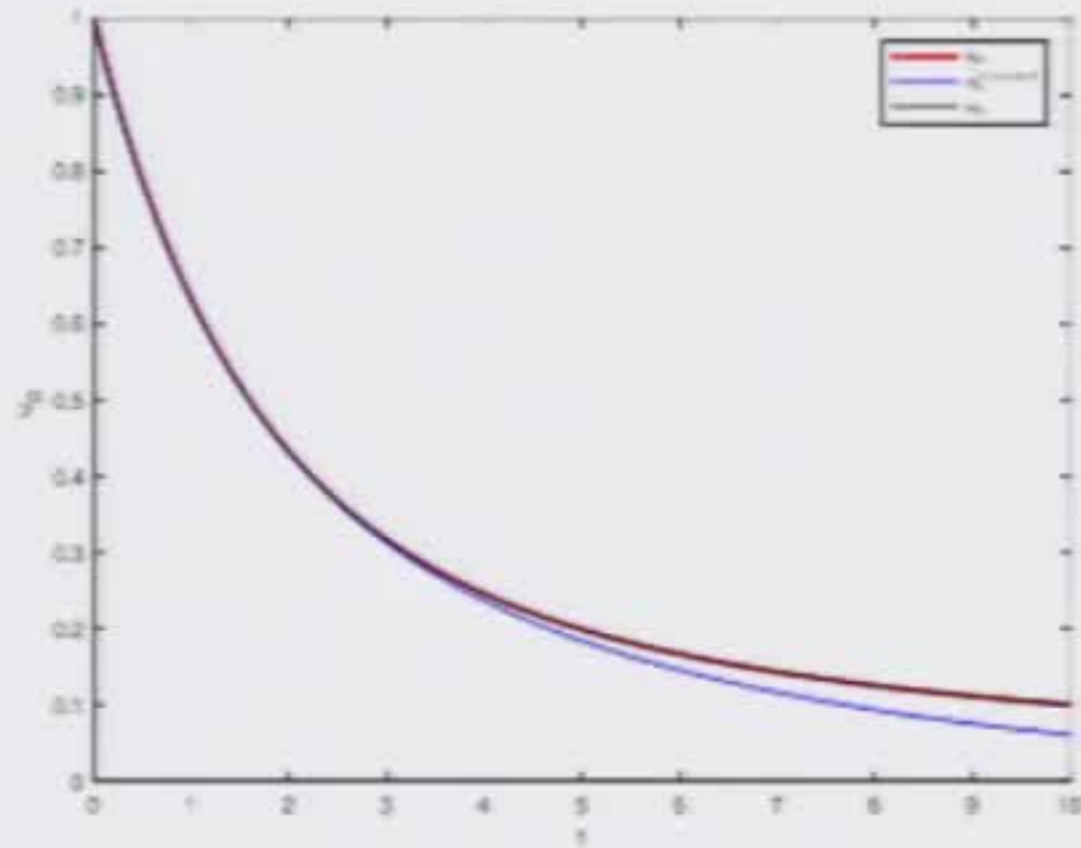
where  $f = w \sin t$  and  $w \sim U(-1, 1)$ . Let  $u \approx \sum_{i=0}^M u_i L_i(w)$ , where  $w \sim U[-1, 1]$  and  $\{L_i\}$  are the Legendre polynomials. We obtain

$$\frac{du_i}{dt} = u_i - \sum_{j,k,m=0}^{P_f} u_j u_k u_m e_{jkmi} + f_i, \quad i = 0, \dots, M, \quad (8)$$

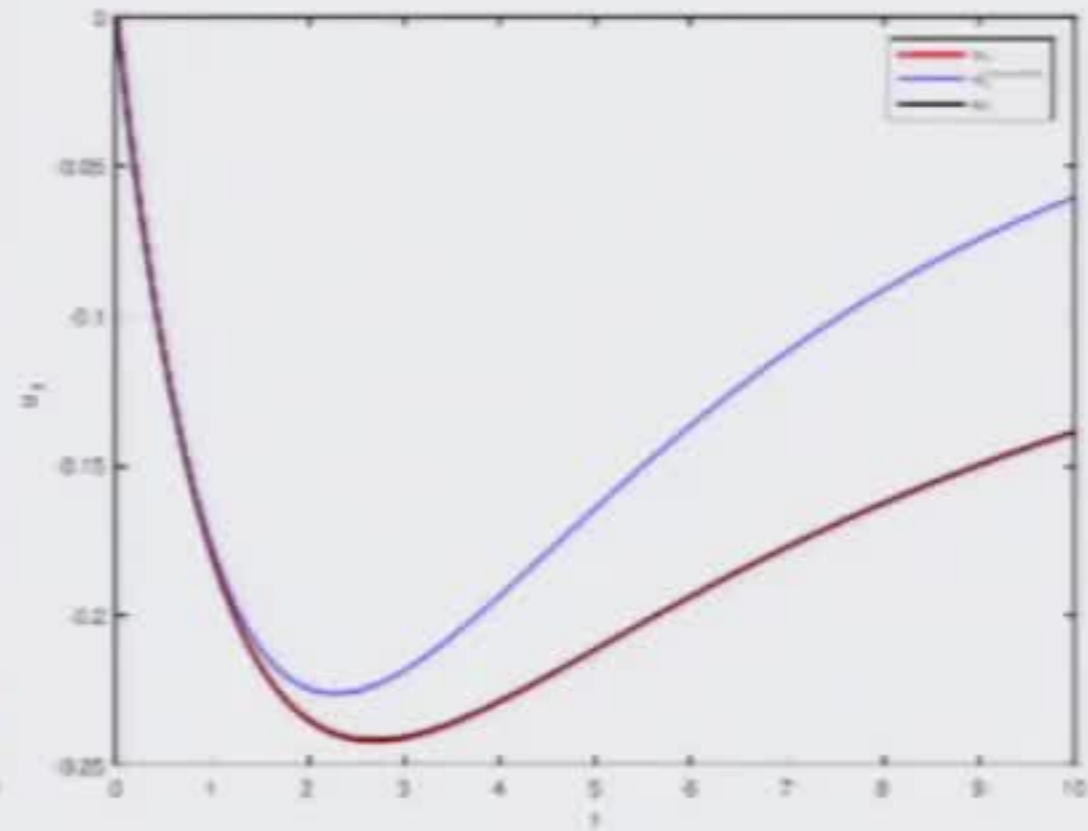
where  $e_{jkmi} = \int_{-1}^1 L_j(w) L_k(w) L_m(w) L_i(w) \frac{1}{2} dw$ .

The projection  $P$  is defined as,  $(Pf)(\hat{u}) = f(\hat{u}, \tilde{0})$ , with  $\hat{u} = (u_0, u_1, \dots, u_\Lambda)$  and  $\tilde{u} = (u_{\Lambda+1}, \dots, u_M)$ .

**Remark:** To compute the memory term in *closed form* we need to introduce a finite-rank projection (in addition to  $P$ ). We use Hermite polynomials as before.



(a)



(b)

**Figure:** Comparison of the solution without memory, with memory and exact solution for the linear equation with uncertain coefficient.

**Remark:** We construct a reduced model with  $\Lambda = 1$  and  $M = 6$ . The model with memory uses 21 basis functions (highest order 5) for the memory term integrand. The integrands for the memory term can be computed by solving Volterra equations.



# Scalar linear differential equation

Consider

$$\frac{du}{dt} = -\kappa u, \quad (5)$$

where  $\kappa \sim U[0, 1]$ . Let  $u \approx \sum_{r=0}^M u_r L_r(w)$ , where  $w \sim U[-1, 1]$  and  $\{L_r\}$  are the Legendre polynomials. We obtain

$$\frac{du_r}{dt} = - \sum_{i=0}^1 \sum_{j=0}^M k_{ijr} u_j, \quad r = 0, \dots, M, \quad (6)$$

where  $e_{ijr} = \int_{-1}^1 L_i(w) L_j(w) L_r(w) \frac{1}{2} dw$ .

The projection  $P$  is defined as,  $(Pf)(\hat{u}) = f(\hat{u}, \tilde{0})$ , with  $\hat{u} = (u_0, u_1, \dots, u_\Lambda)$  and  $\tilde{u} = (u_{\Lambda+1}, \dots, u_M)$ .

**Remark:** To compute the memory term in *closed form* we need to introduce a finite-rank projection (in addition to  $P$ ). We use

$$(P' \varphi_j)(\hat{u}, t) \approx \sum_{\nu} (\varphi_j(u, t), h^{\nu}(\hat{u})) h^{\nu}(\hat{u}),$$

where  $h^{\nu}$  are Hermite polynomials.