Structure preserving model reduction on Lie groups

Geometric Numerical Integration – MFO

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March 21–25, 2016

Outline

1. *Model reduction in* $\mathbb{R}^N$
2. *Model reduction for mechanical systems*
3. *Model reduction for mechanical systems on Lie groups*
4. *Dipole example, water molecules*
5. *Numerical experiments*

- Very large dynamical systems are complicated both to analyse and to do computations on
- In many cases, for instance in mechanical systems, one can find a low dimensional space in which most of the [interesting] dynamics take place
- By model reduction, we mean a procedure for constructing this lower dimensional space, and mapping the dynamics (differential equations) onto this space
- For mechanical systems we would like the structural properties of the high-dimensional system to be preserved after the reduction.

$$\dot{y} = f(y), \qquad y \in \mathbb{R}^N, \quad N \text{ very large}$$

Use the following procedure

1. Compute a sample trajectory by a numerical method to generate $\{y^k\},\ k = 1, 2, \ldots$.
2. Compute an (approximate) SVD

$$[y_0, \cdots] = \bar{U}\Sigma\bar{V}^T$$

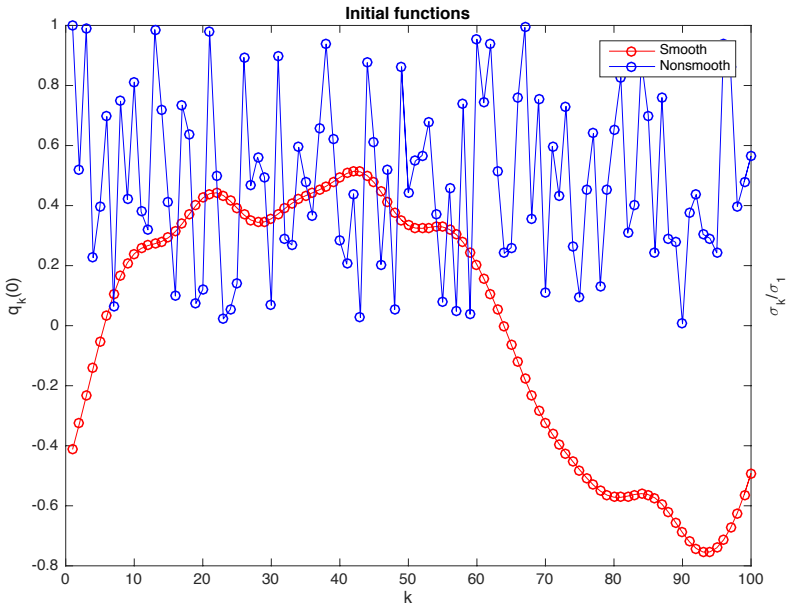
3. for $\sigma_{n+1} < \texttt{tol}$, set $U = \bar{U}(:,1{:}n)$.
4. Define $y = Uz$ and solve

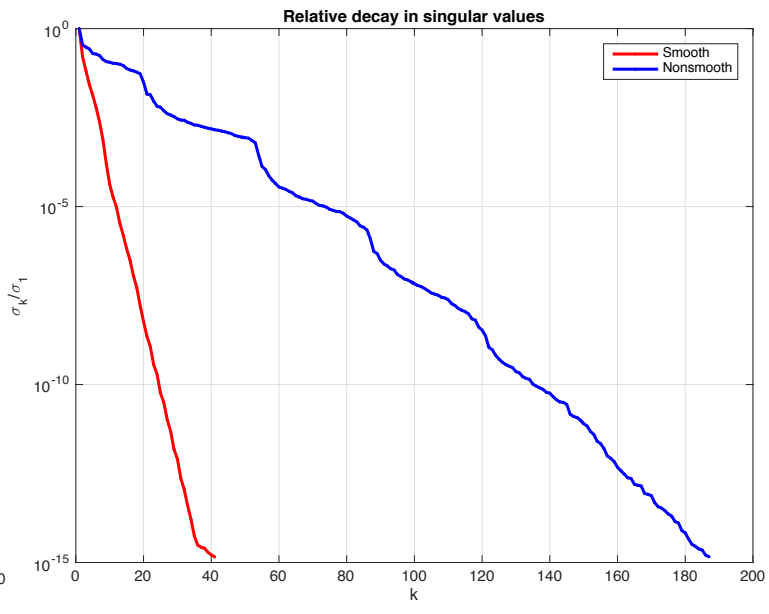
$$\dot{z} = U^T f(Uz), \quad \text{for } z \in \mathbb{R}^n$$

Hopefully $n \ll N$ and $y(t) \approx Uz(t)$.

Example

$$H(q,p) = \frac{1}{2}p^T p + \sum_{i=1}^{N} \frac{1}{2}(q_{i+1} - q_i)^2 + \frac{\beta}{4}(q_{i+1} - q_i)^4$$





Suppose $L : TM \to \mathbb{R}$ is a Lagrangian. Variational principle leads to Euler-Lagrange equations

$$\delta \int_a^b L(q(t), \dot{q}(t))\,\mathrm{d}t = 0 \quad \Rightarrow \quad \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} = \frac{\partial L}{\partial q}$$

Natural Lagrangians are those of the form

$$L(q, \dot{q}) = \frac{1}{2}\langle M\dot{q}, \dot{q}\rangle - V(q)$$

for which the Euler-Lagrange equations are

$$M\ddot{q} = -DV(q), \quad p = M\dot{q}$$

Suppose the SVD has been performed *only on* the q-part, so that

$$q = UQ, \qquad \dot{q} = U\dot{Q}$$

Then the reduced Lagrangian is

$$\bar{L}(Q, \dot{Q}) = \frac{1}{2}\langle MU\dot{Q}, U\dot{Q}\rangle - V(UQ)$$

and the corresponding Euler-Lagrange equations are

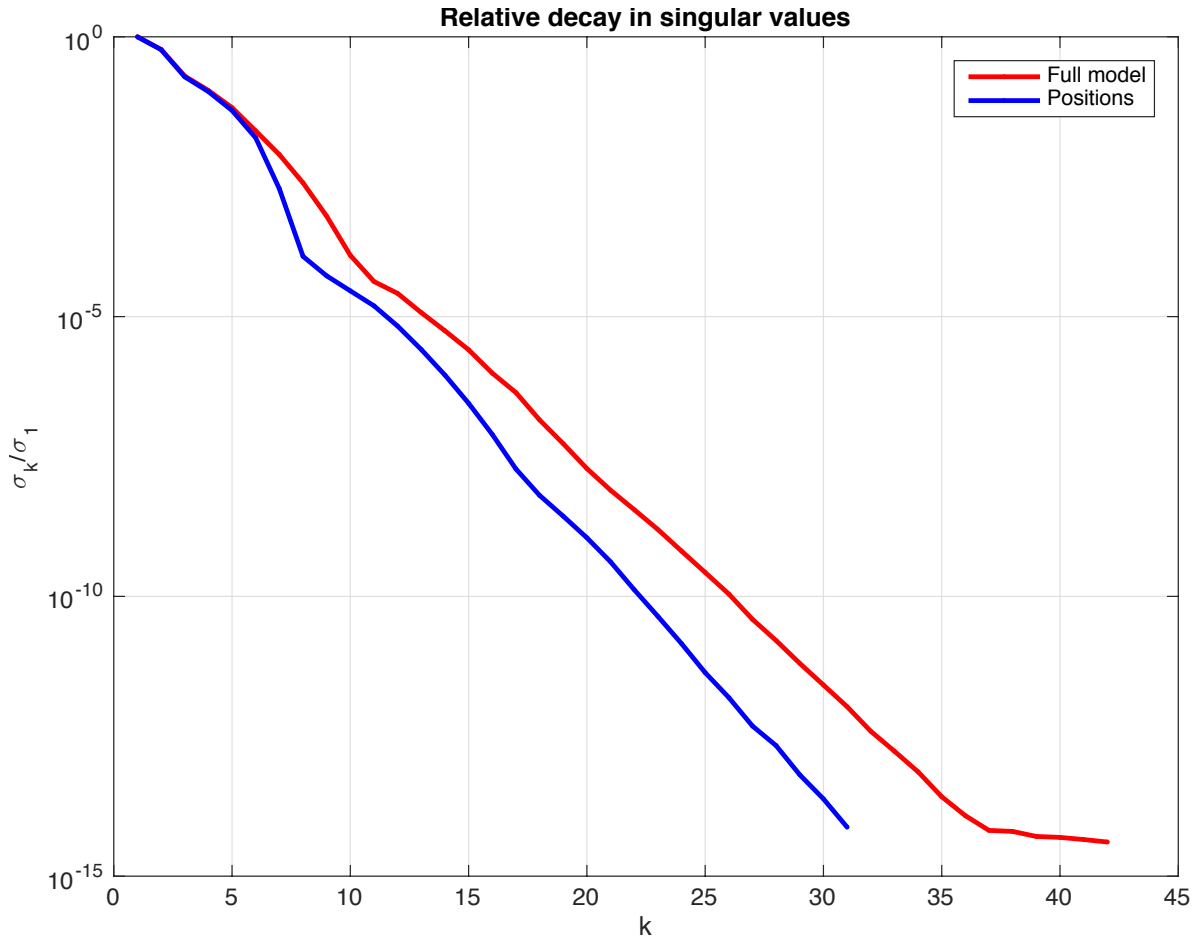
$$U^T MU\ddot{Q} = -U^T DV(UQ)$$

The Legendre transform is $\Pi = \bar{M}\dot{Q} = U^T MU\dot{Q}$ and

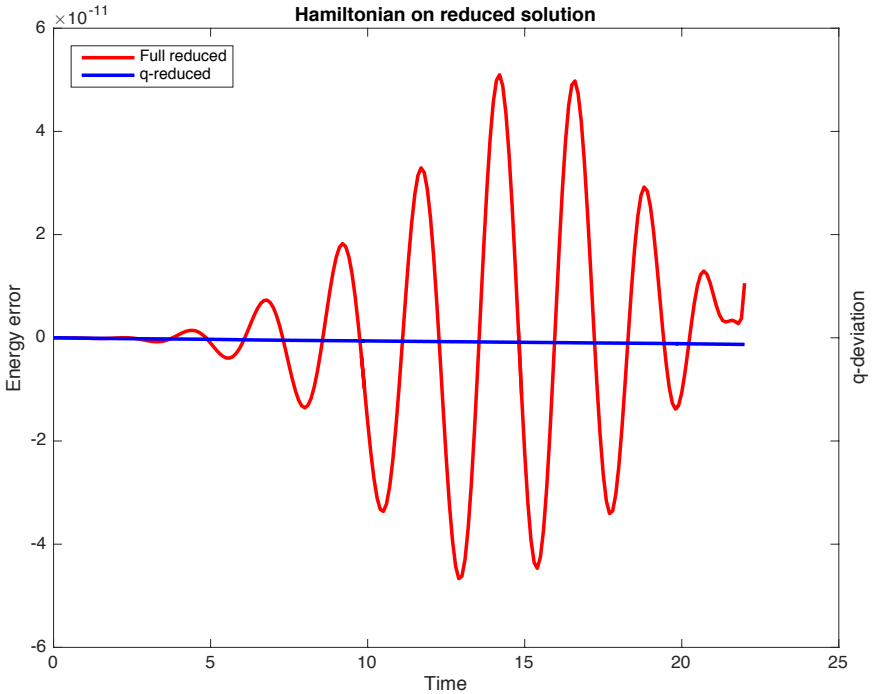
$$H(Q, \Pi) = \frac{1}{2}\langle \Pi, \bar{M}^{-1}\Pi\rangle + V(UQ)$$

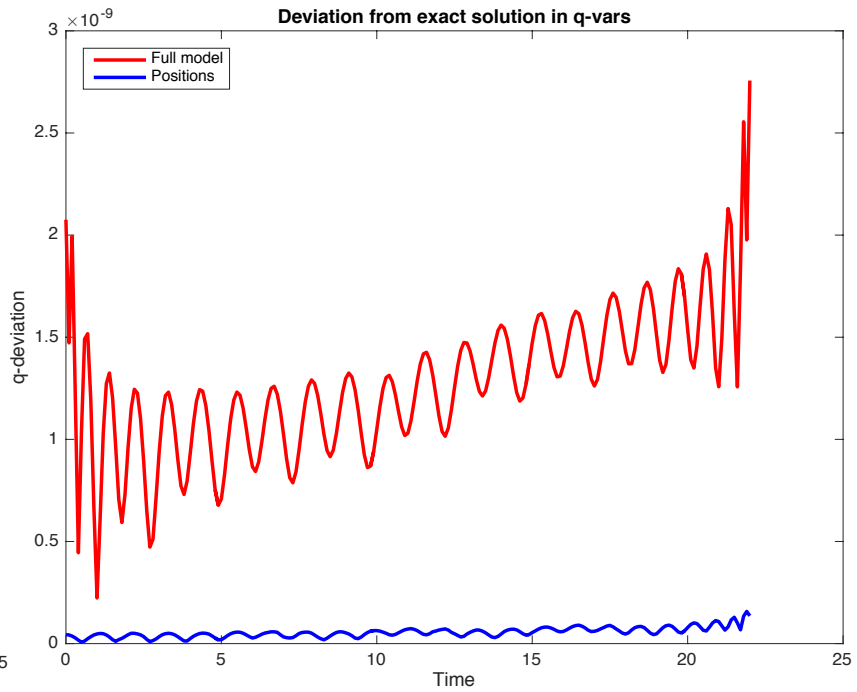
Example revisited

The reduction on q *only* paves the way for structure preserving reduced models



Example – Structure preserving works better





Note: We are only computing "exact solutions" here

Most Lie group integrators employ either

1. Local coordinates on the group or
2. a global embedding of the group into a Euclidean model space

Both these choices have difficulties

1. The idea of model reduction is to create a subspace through sampling of (large) portions of phase space. It is challenging to handle the switching between charts. Exampe: If $SO(3)^N$ is employed, then at least 4^N charts are needed.
2. Global coordinates are difficult because the reduction procedure does not respect the constraints

The following procedure was proposed

1. Given a configuration manifold Q, embed it into some linear space V
2. Apply reduction to problem in V and obtain reduced linear space $V_r \subset V$.
3. Construct the reduced manifold Q_r as $Q_r = V_r \cap Q$.

Problem:

$$\dim V_r = \dim Q_r + \dim V - \dim Q$$

This scales badly for large scale problems.

- G Lie group with tangent bundle TG, Lie algebra $\mathfrak{g} \simeq T_eG$
- $L : TG \to \mathbb{R}$ is Lagrangian, $L(q, \dot{q})$
- Left trivialized L is $\ell : G \times \mathfrak{g} \to \mathbb{R}$

$$\ell(g, \xi) = L(g, g\xi)$$

Hamilton–Pontryagin variational principle

$$\delta \int_a^b [\ell(g, \xi) + \langle \mu, g^{-1}\dot{g} - \xi \rangle] \, \mathrm{d}t = 0$$

where $g \in G$, $\xi \in \mathfrak{g}$ and $\mu \in \mathfrak{g}^*$ are varied freely and independently.

$$\frac{\partial \ell}{\partial \xi} = \mu, \qquad g^{-1}\dot{g} = \xi$$

$$L_g^* g \frac{\partial \ell}{\partial g} = \dot{\mu} - \mathrm{ad}_\xi^*(\mu)$$

Hamilton–Pontryagin in local coordinates

We introduce the local Lagrangian (near $g_0 \in G$)

$$\tilde{\ell}(v, w) = \ell(g_0 \exp(v), \operatorname{dexp}_v(w))$$

where $\operatorname{dexp}_v : \mathfrak{g} \to \mathfrak{g}$ is

$$\operatorname{dexp}_v(w) = L_{\exp(-v)*} \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} \exp(v + \varepsilon w)$$

It is well-known that

$$\operatorname{dexp}_v = \left.\frac{1 - \exp(-z)}{z}\right|_{z=\operatorname{ad}_v}$$

Local Hamilton–Pontryagin principle

$$\delta \int_a^b [\tilde{\ell}(v, w) + \langle \tilde{\mu}, \dot{v} - w \rangle] \, \mathrm{d}t = 0$$

where $v, w, \tilde{\mu}$ are varied freely and independently.

The resulting equations in local coordinates are

$$\frac{\partial \tilde{\ell}}{\partial w} = \tilde{\mu}$$
$$\dot{v} = w$$
$$\frac{\partial \tilde{\ell}}{\partial v} = \frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mu}$$

Proposition

The equations derived from the Hamilton-Pontryagin principle for $v, w, \tilde{\mu}$ are locally equivalent to the equations derived from the Hamilton-Pontryagin principle in terms of g, ξ, μ.

Construct as usual a reduced basis U via SVD to the full system in local coordinates. Use the approximations

$$v \approx U\lambda, \qquad w \approx U\eta$$

to define the reduced Lagrangian

$$\tilde{\ell}_r(\lambda, \eta) = \ell\big(g_0 \exp(U\lambda), \operatorname{dexp}_{U\lambda}(U\eta)\big)$$

and employ, yet again, the HP-principle

$$\delta \int_a^b [\tilde{\ell}(U\lambda, U\eta) + \langle U\gamma, U\dot{\lambda} - U\eta\rangle]\, \mathrm{d}t = 0$$

λ, η, γ varied freely, and independently

Found e.g. in Dullweber et al. (1997).
We consider a Hamiltonian system for d soft dipolar spheres. The configuration manifold is the Lie group $G = (SO(3) \times \mathbb{R}^3)^{\times d}$.

$$H(q, p, m, Q) = T(p, m) + V(q, Q)$$

$$T(p, m) = \sum_{i=1}^{d} \frac{1}{2}\|p_i\|^2 + \frac{1}{2}\langle m_i, I_i^{-1} m_i \rangle$$

The potential is the sum of a short range and dipole potential.

$$V(q, Q) = V^s(q) + V^d(q, Q)$$

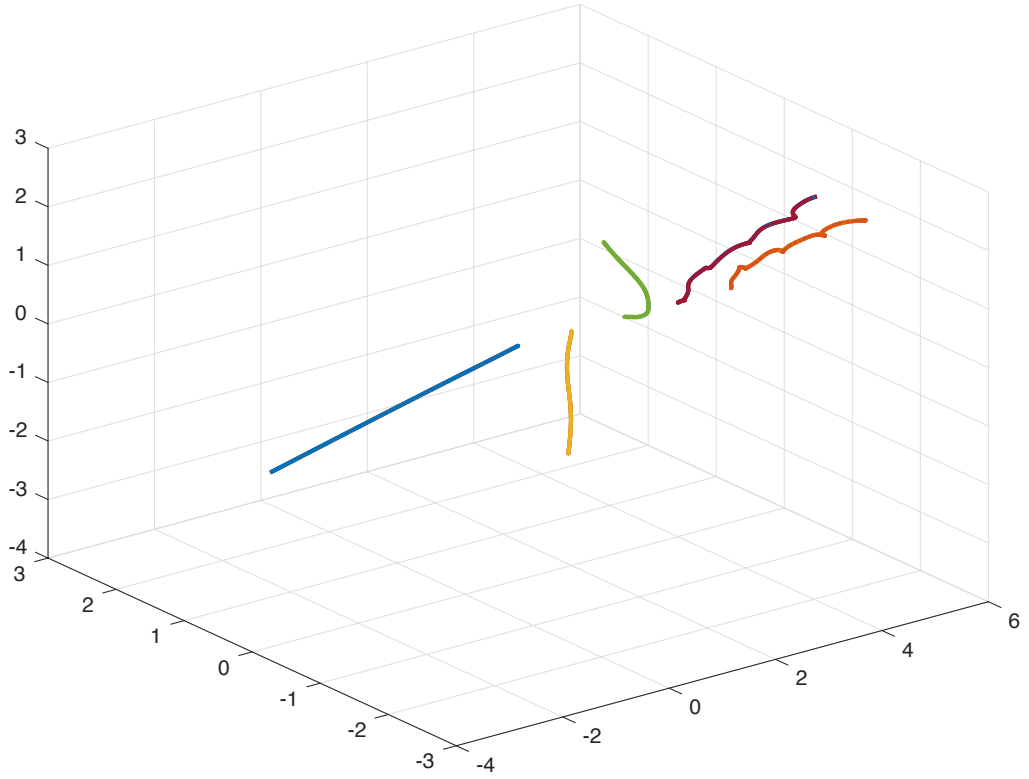
$$V^s(q) = 4\epsilon \sum_{j>i} \left(\frac{\sigma}{|r_{ij}|} \right)^{12}, \quad r_{ij} = q_i - q_j$$

Dipole potential

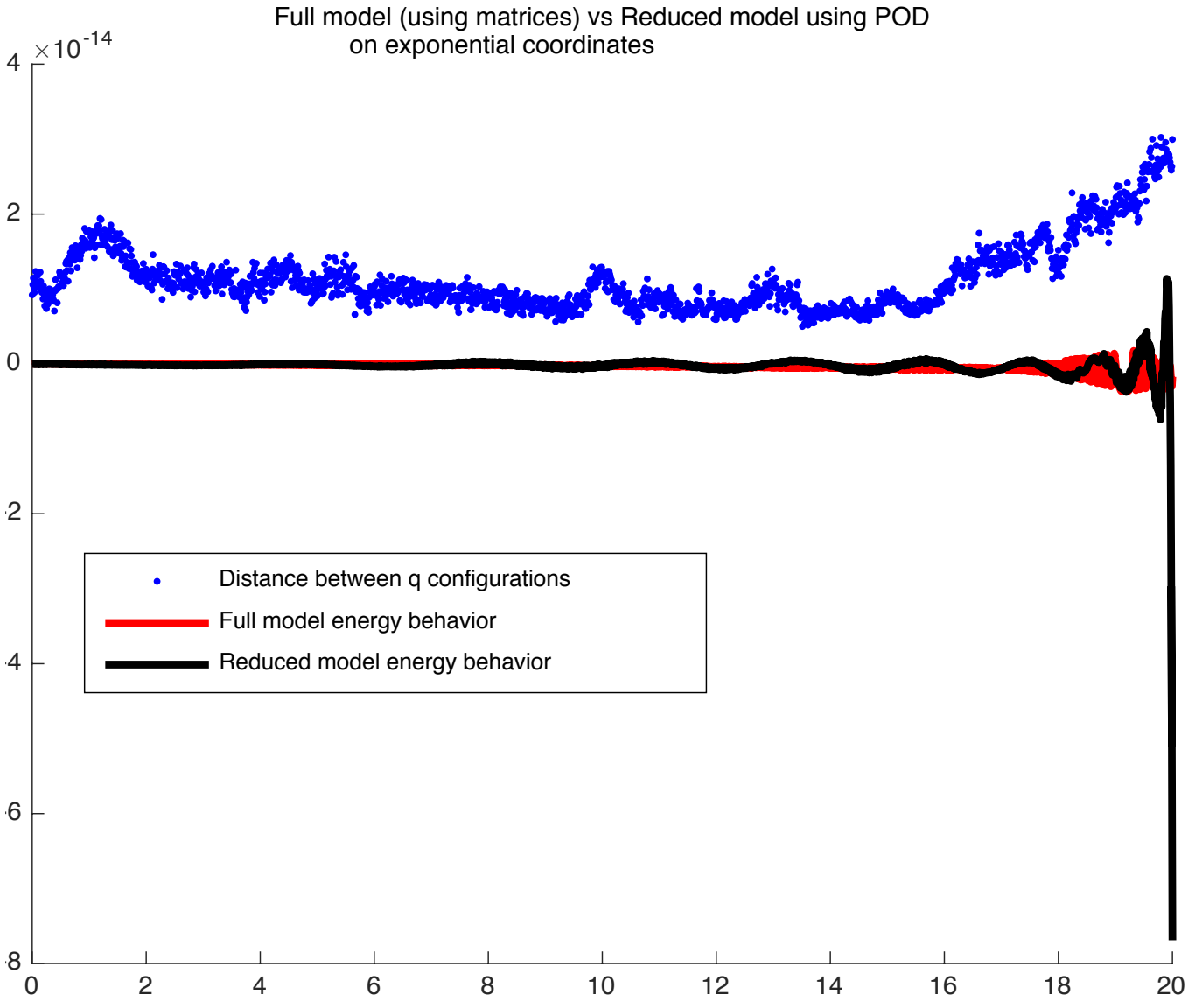
$$V^d = \sum_{j>i} \frac{1}{|r_{ij}|^3} \mu_i \cdot \mu_j - \frac{3}{|r_{ij}|^5} (\mu_i \cdot r_{ij})(\mu_j \cdot r_{ij})$$

where

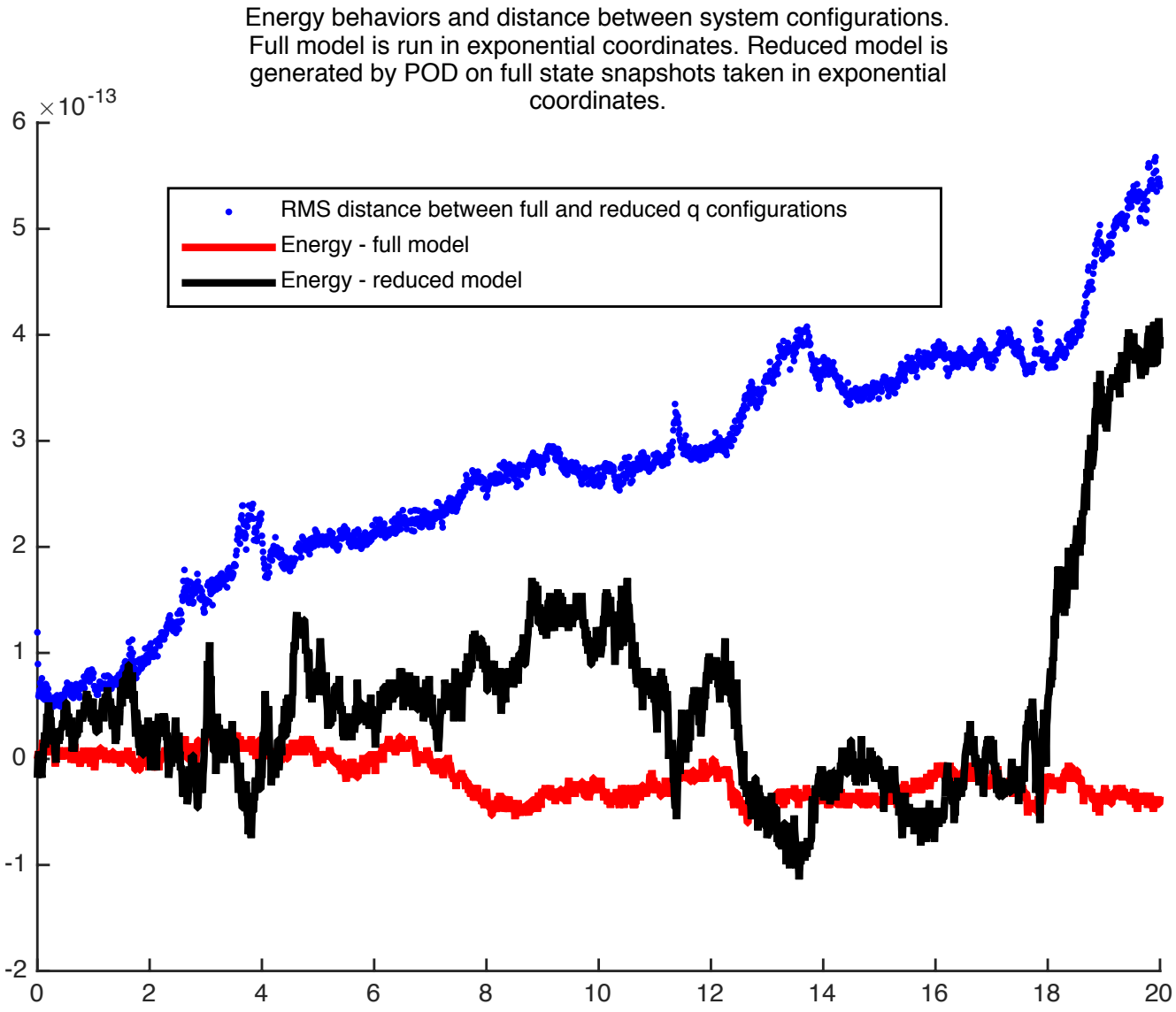
$$\mu_i = Q_i \bar{\mu}_i, \qquad \bar{\mu}_i \text{ fixed reference orientation of molecule } i$$



Numerical experiment – dipole



Numerical experiment – dipole 30 molecules



- It is not entirely satisfactory that our current method cannot switch between charts in a geometric manner
- Recently, in shape analysis one has started to use some results by Kriegl and Michor related to an isomorphism between smooth curves in the Lie algebra and smooth curves on the corresponding Lie group
- This allows for global representations of entire curves

Some references

1. S. Lall, P. Krysl, J. E. Marsden, *Structure-preserving model reduction for mechanical systems*, Physica D 184 (2003) 304–318.
2. A. Dullweber, B. Leimkuhler, R. McLachlan, *Symplectic splitting methods for rigid body molecular dynamics*, J. Chem. Phys. 107 (1997) 5840–5851.
3. E. Celledoni, F. Fassò, N. Säfstrøm, A. Zanna, *The exact computation of the free rigid body motion and its use in splitting methods*, SIAM J. Sci. Comput. 30 (2008) 2084–2112.

Thanks for your attention!