QUIET 2017

Structure preserving reduced order modeling

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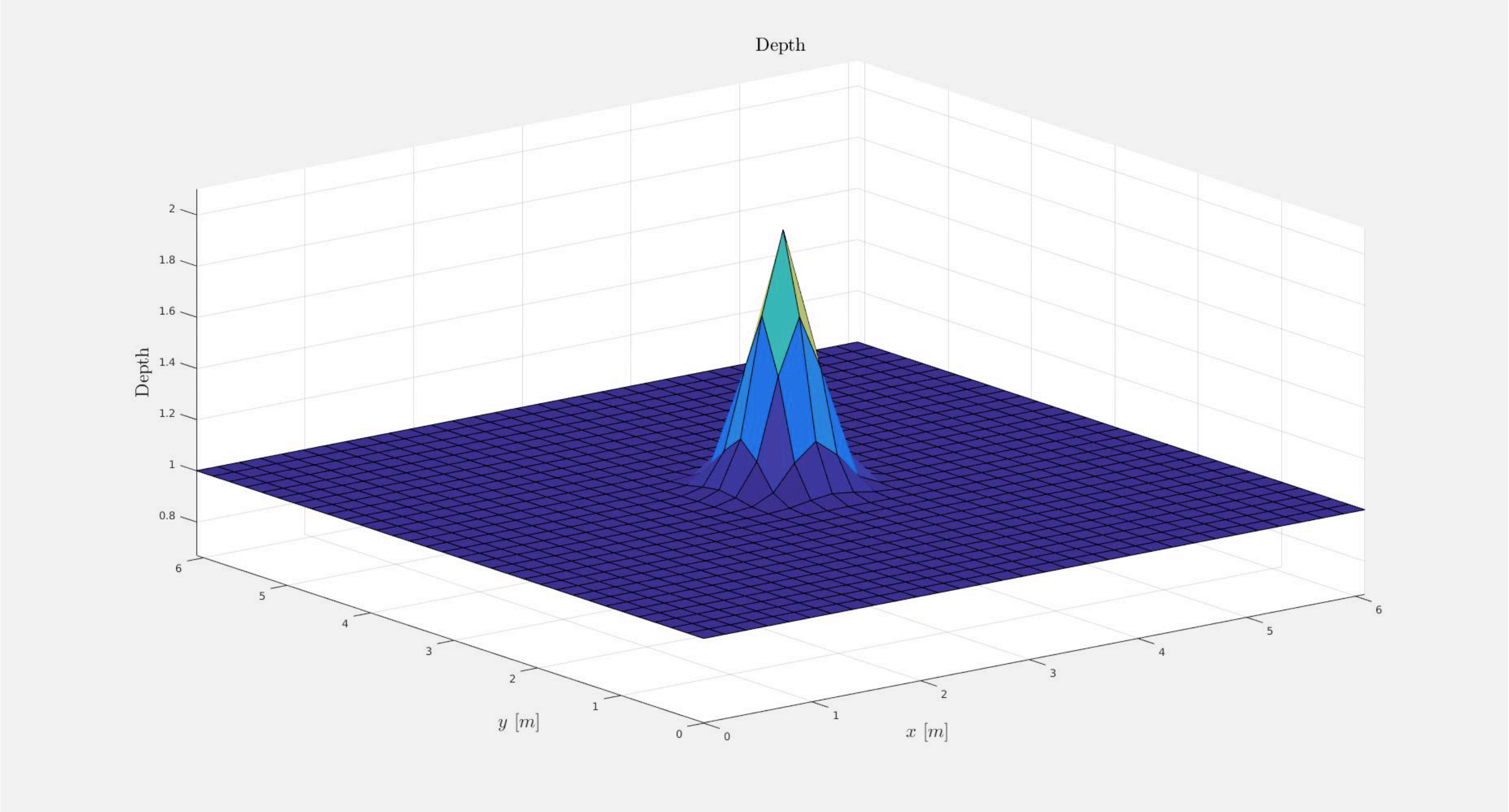

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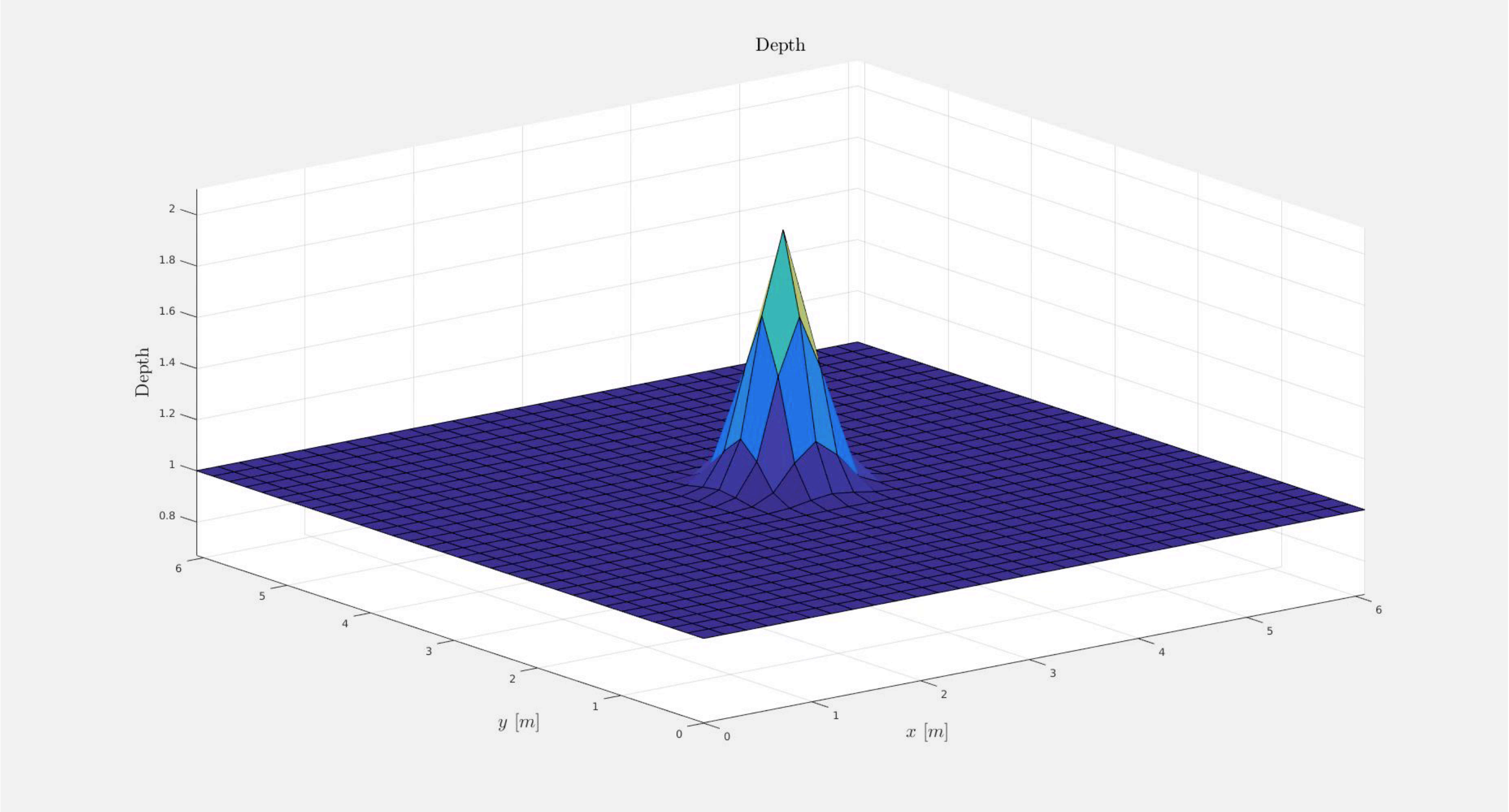

Model order reduction

Let us consider ODE's (or semi-discrete PDE's) as

$$\begin{cases} \mathbf{z}(\mu)_t = L(\mu)\mathbf{z}(\mu) + F(\mu, \mathbf{z}(\mu)) \\ \mathbf{z}(\mu, 0) = \mathbf{z}_0(\mu) \end{cases}$$

where

$$\mathbf{z} \in \mathcal{R}^n \qquad n \gg 1$$

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$$\mathbf{z} \in \mathcal{R}^n \qquad n \gg 1$$

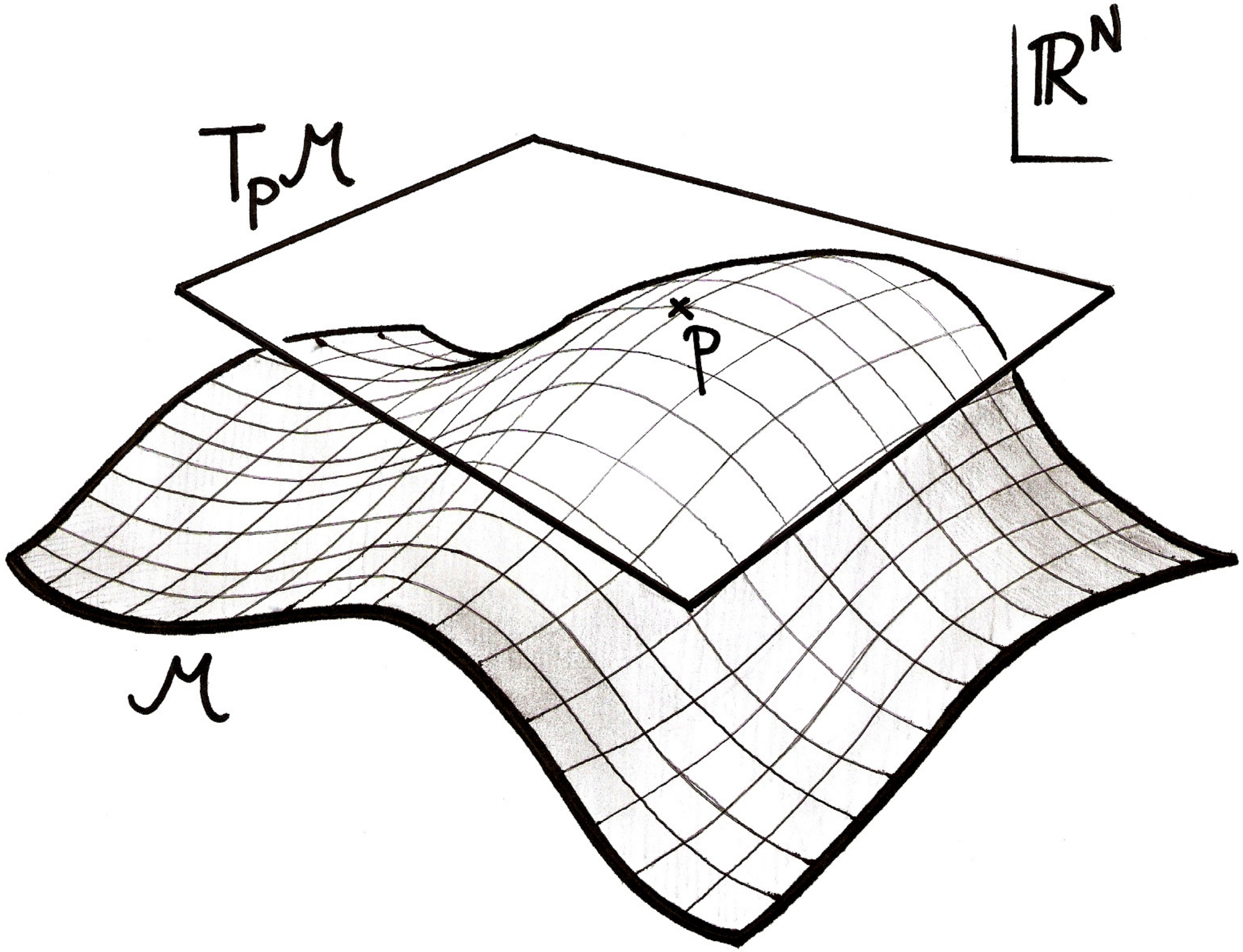
Now we seek the reduced model

$$\mathbf{z} = \mathrm{A}\mathbf{y}$$

where $\mathbf{y} \in \mathcal{R}^k \qquad \mathrm{A} \in \mathcal{R}^{n \times k} \qquad n \gg k$

Model order reduction

We seek a linear approximation to the solution manifold



Model order reduction

By projection, we obtain the reduced system

$$\begin{cases} \mathrm{A}\mathbf{y}(\mu)_t = L(\mu)\mathrm{A}\mathbf{y}(\mu) + F(\mu, \mathrm{A}\mathbf{y}(\mu)) \\ \mathrm{A}\mathbf{y}(\mu, 0) = \mathrm{A}\mathbf{y}_0(\mu) \end{cases}$$

$$\mathrm{A}^{+}\mathrm{A} = \mathrm{I}$$

and

$$\begin{cases} \mathbf{y}(\mu)_t = \mathrm{A}^{+}L(\mu)\mathrm{A}\mathbf{y}(\mu) + \mathrm{A}^{+}F(\mu, \mathrm{A}\mathbf{y}(\mu)) \\ \mathbf{y}(\mu, 0) = \mathbf{y}_0(\mu) \end{cases}$$

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Choosing the linear space - A - is clearly key

Often done by accuracy

- POD
- Greedy approximation based on error

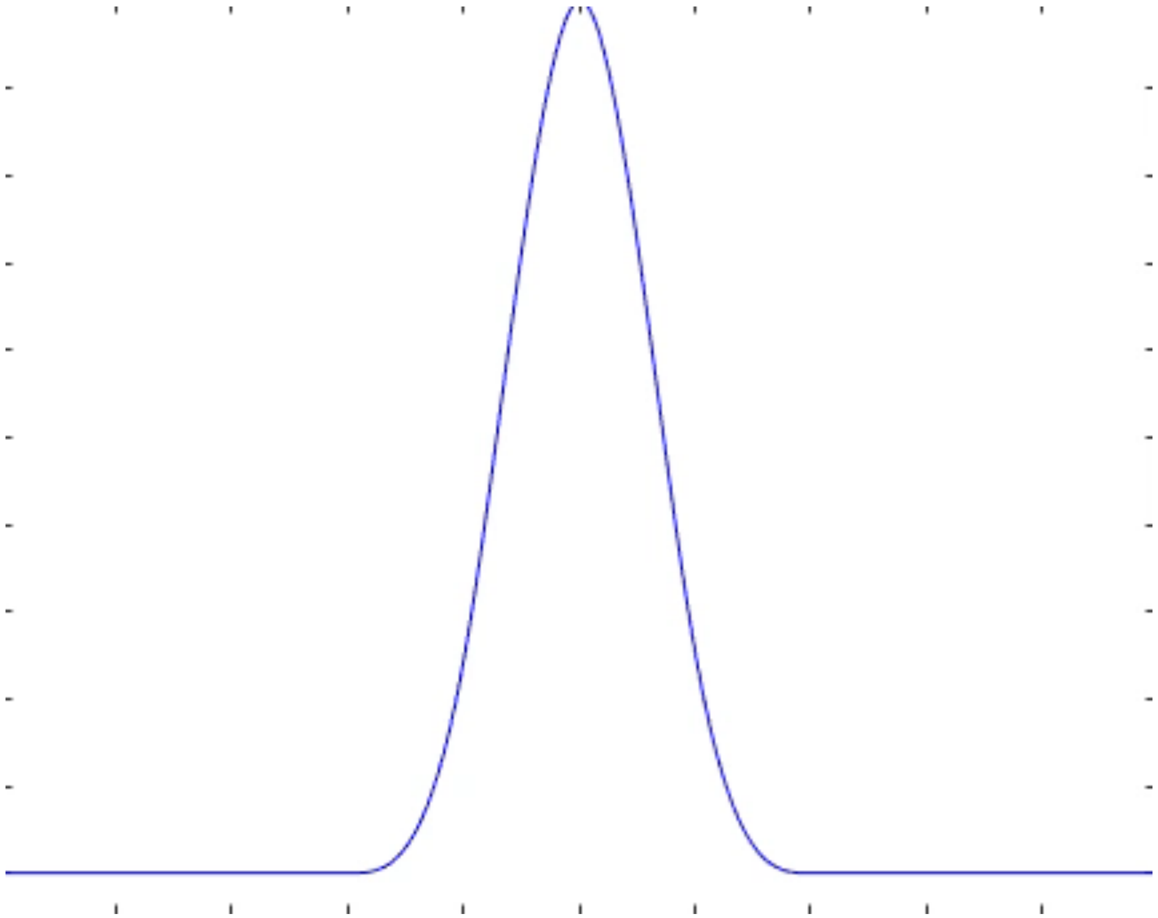
A known problem

Consider the wave equation

$$u_{tt} - c^2 u_{xx} = 0$$

Expressed as

$$\begin{cases} q_t = p \\ p_t = c^2 q_{xx} \end{cases}$$



Reduced model by POD

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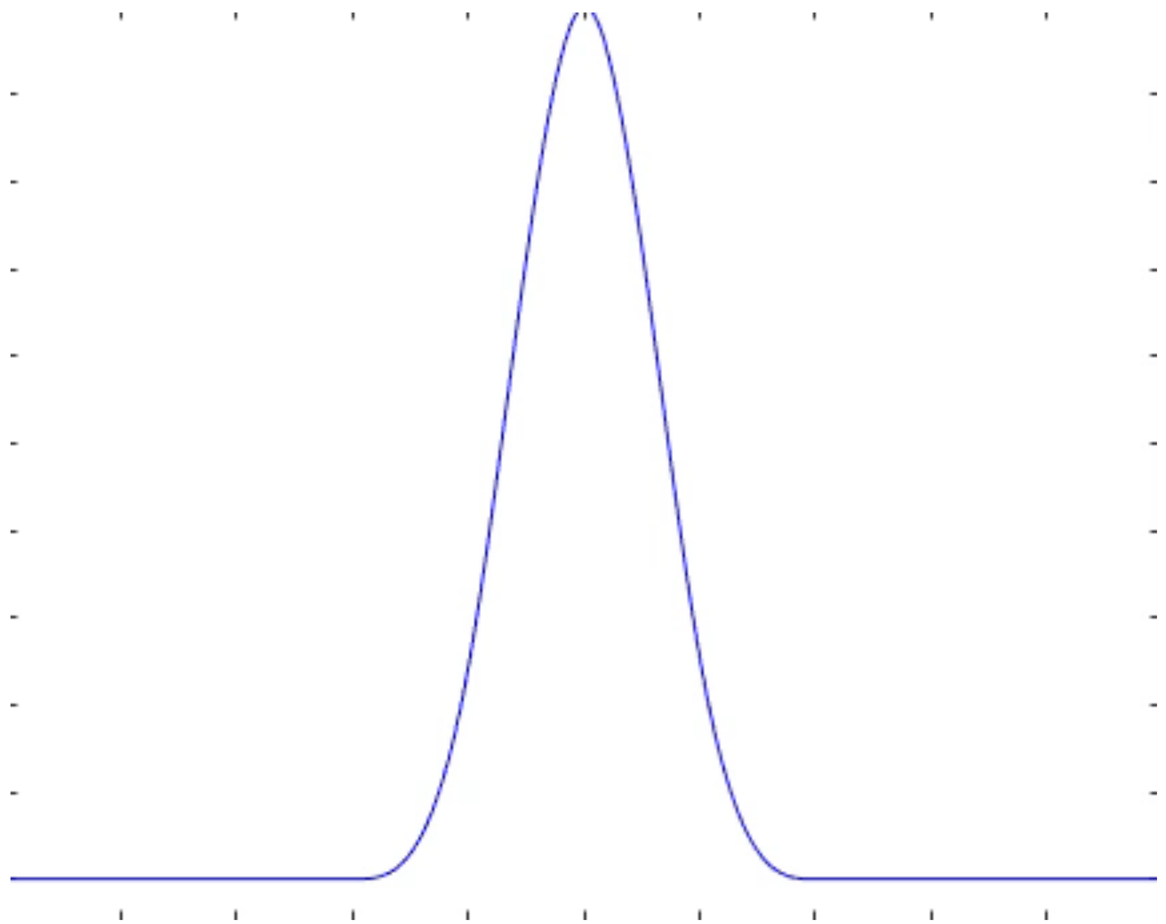

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Consider shallow water equation

$$\begin{cases} h_t + \nabla \cdot (h \nabla \phi) = 0 \\ \phi_t + \frac{1}{2} |\nabla \phi|^2 + h = 0 \end{cases}$$

$$\mathbf{u} = \nabla \phi$$

A known problem

k=80

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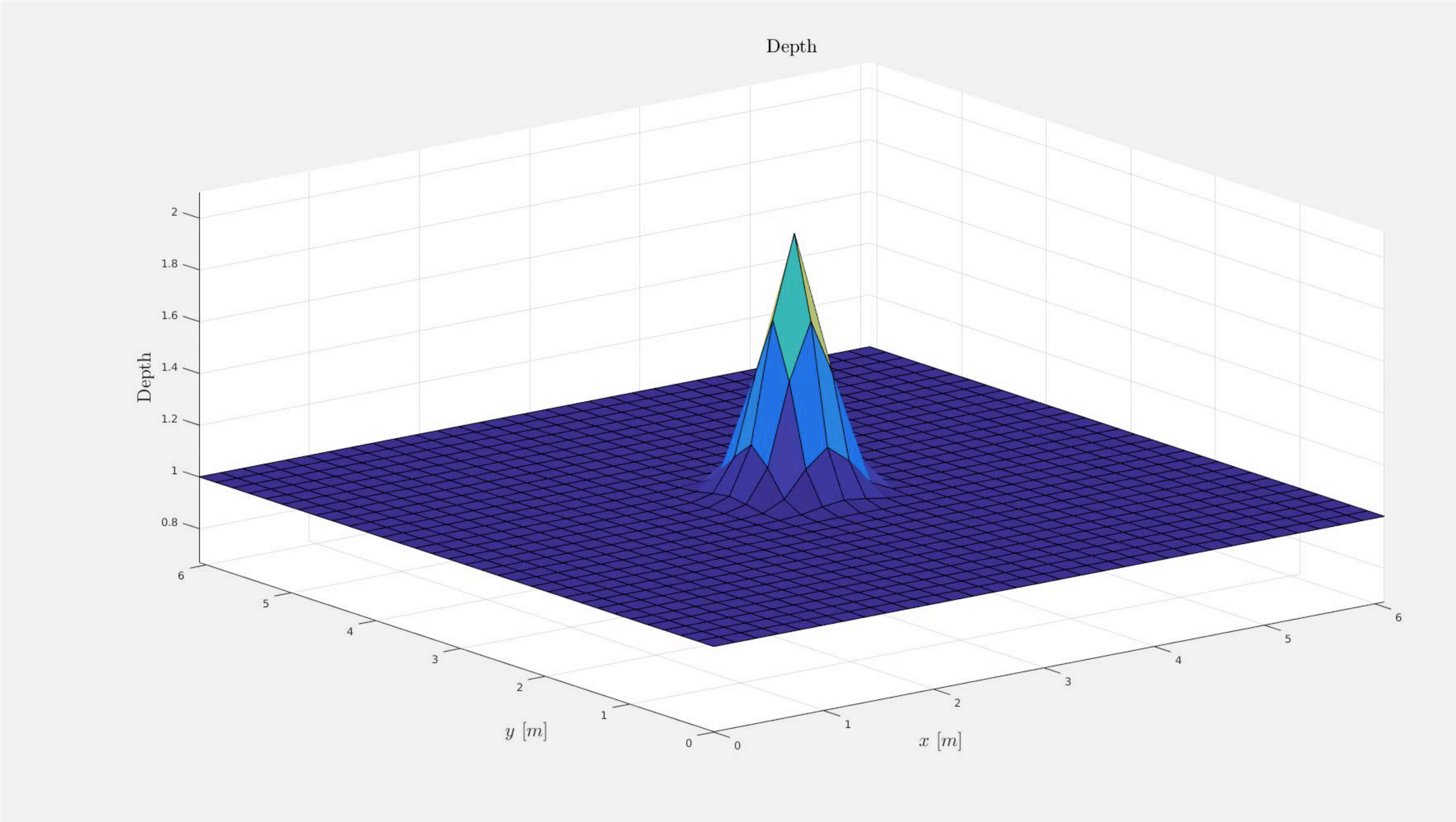

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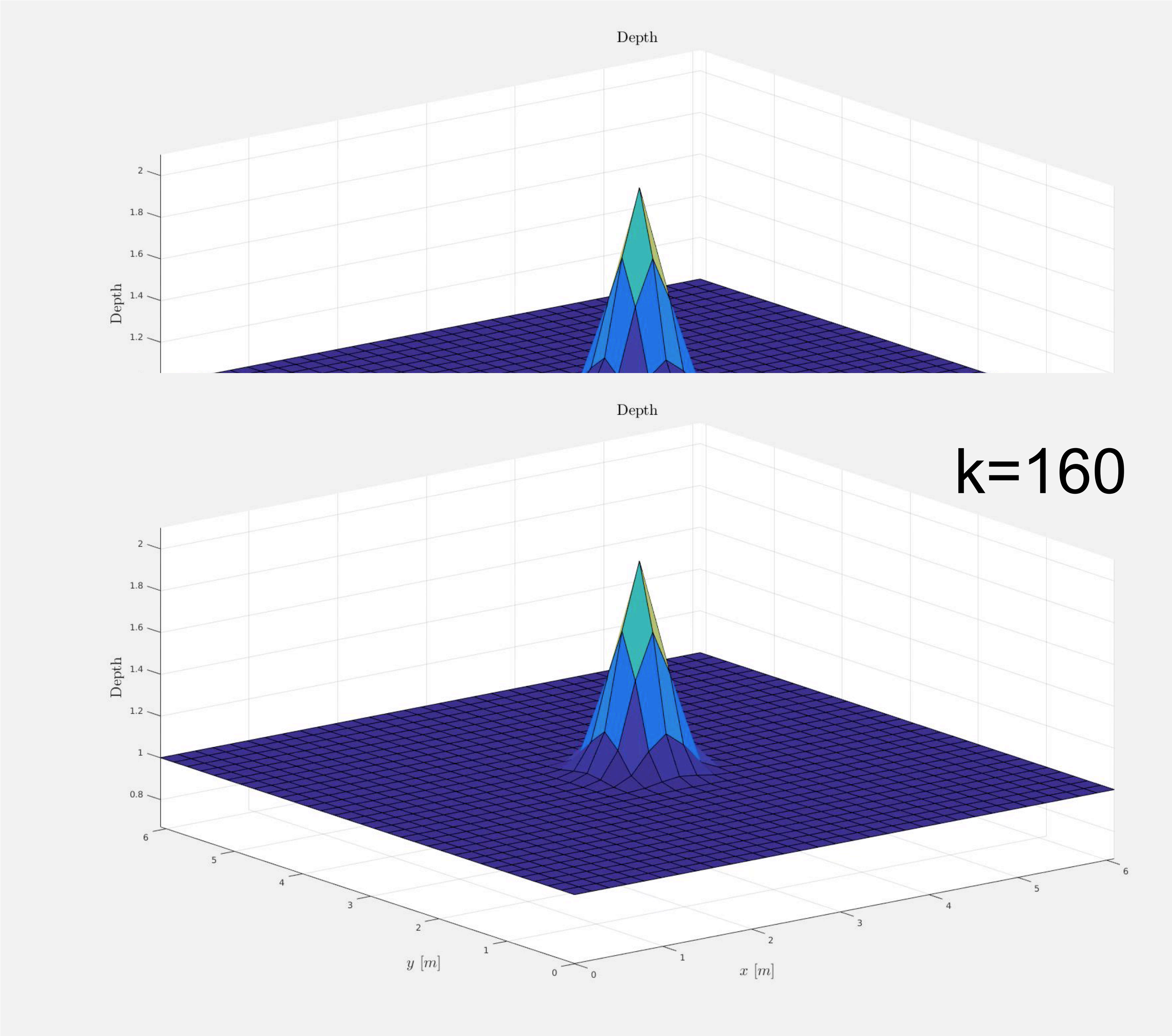

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Mode truncation instability

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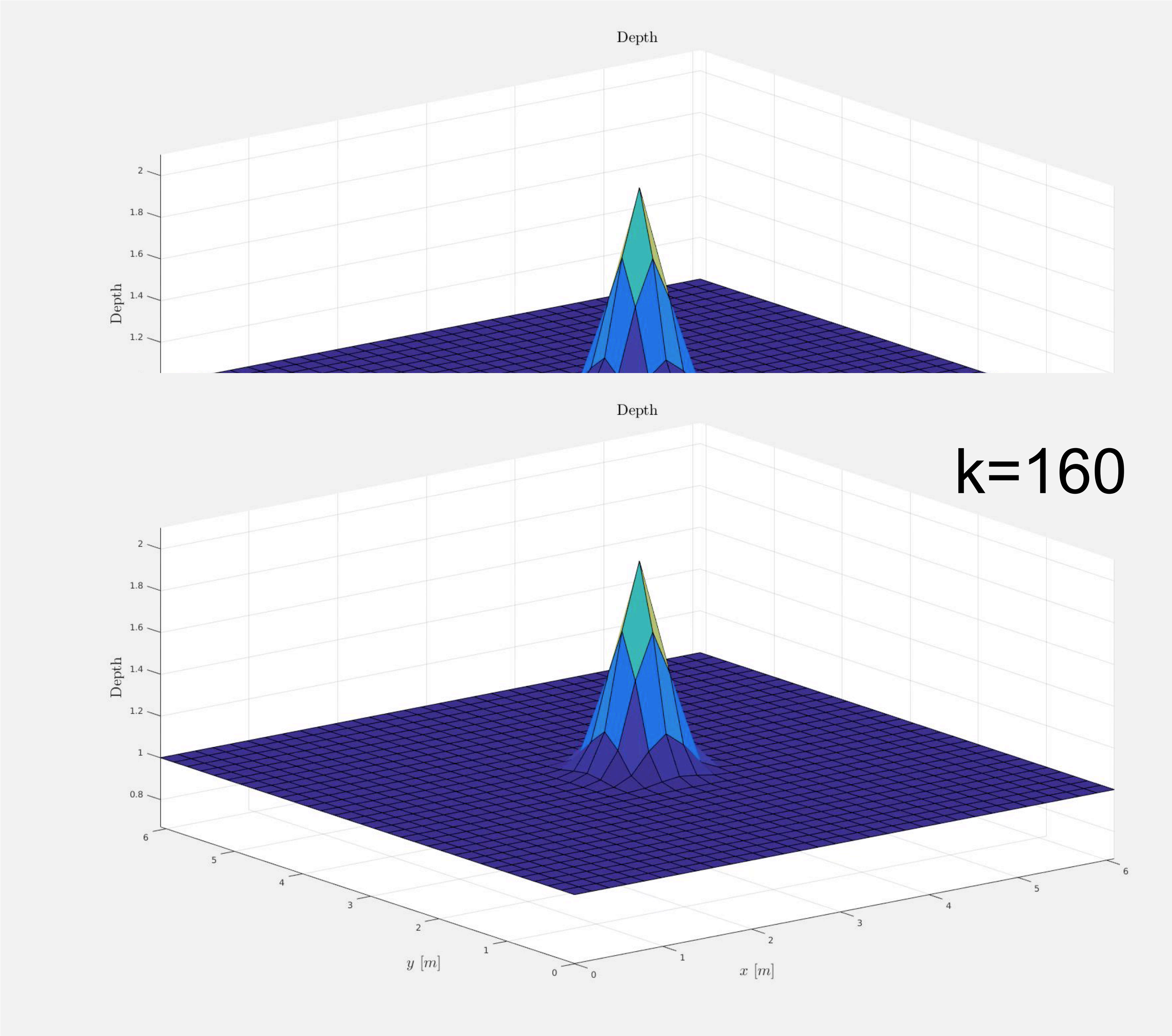

Reduced model by POD

Problem ?

Problem - we have destroyed delicate properties

Systems are Hamiltonian

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Systems are Hamiltonian

Equations of evolution,

$$\begin{cases} \dot{\mathbf{q}} = \dfrac{dH}{d\mathbf{p}} \\ \dot{\mathbf{p}} = -\dfrac{dH}{d\mathbf{q}} \end{cases}$$

Or by defining $\mathbf{y} = \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}$

$$\dot{\mathbf{y}} = \mathbb{J}_{2n} \nabla_{\mathbf{y}} H(\mathbf{y}) \qquad \mathbb{J}_{2n} = \begin{bmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{bmatrix}$$

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We must develop our reduced basis such that the reduced model maintains a Hamiltonian structure

Model order reduction

Definition: $A \in \mathbb{R}^{2n \times 2k}$ *is a symplectic basis/transformation if:*

$$A^T \mathbb{J}_{2n} A = \mathbb{J}_{2k}$$

Definition: *A set* $\mathcal{A}$ *of vectors*

$$\mathcal{A} = \{e_1, \dots, e_n\} \cup \{f_1, \dots, f_n\}$$

is a symplectic basis if

$$\Omega(e_i, e_j) = \Omega(f_i, f_j) = 0, \quad \Omega(f_i, e_j) = \delta_{i,j}$$

$$\Omega(v_1, v_2) = v_1^T \mathbb{J}_{2n} v_2$$

Symplectic transformations

Symplectic Transformation:

- A symplectic inverse of a symplectic matrix A is given by

$$A^+ = \mathbb{J}_{2k}^T A^T \mathbb{J}_{2k}$$

- If A is a symplectic matrix then (Peng et al. [2015])
  - $(A^+)^T$ is symplectic
  - $A^+ A = I_{2k}$

Model order reduction

Suppose for a symplectic subspace

$$z \approx Ay, \qquad A \in \mathbb{R}^{2n \times 2k}$$

With substitution

$$A\dot{y} = \mathbb{J}_{2n} \nabla_z H(Ay)$$

We require the residual be orthogonal to A:

$$A^+ \left(A\dot{y} - \mathbb{J}_{2n} \nabla_z H(Ay) \right) = 0$$

resulting

$$\dot{y} = \underbrace{A^+ \mathbb{J}_{2n} (A^+)^T}_{\mathbb{J}_{2k}} \nabla_y \tilde{H}(y), \quad \tilde{H}(y) = H(Ay)$$

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Since A is symplectic, reduced problem is symplectic

Reduced models

Given set of Snapshots $Y = [\mathbf{y}(t_1), \ldots, \mathbf{y}(t_N)]$

- Nonlinear optimization

$$\underset{A}{\text{minimize}} \quad ||Y - AA^+Y||$$
$$\text{subject to} \quad A^T \mathbb{J}_{2n} A = \mathbb{J}_{2k}$$

- SVD based methods for basis generation.
- Complex SVD, using $\mathbf{q} + i\mathbf{p}$.
- Greedy approach.

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The Hamiltonian can be used as error estimator.

$$H(\mathbf{q}, \mathbf{p}) = U(\mathbf{q}) + K(\mathbf{p}) = F_1(\mathbf{q}, \mathbf{p}) + F_2(\mathbf{q}, \mathbf{p})$$

The greedy method - error

Let $\hat{z}(t) := Ay(t)$ be the approximated solution. Energy loss associated with model reduction is

$$\Delta H(t) := |H(z(t)) - H(\hat{z}(t))|$$

Now we have

$$\begin{aligned}
H(\hat{z}(t)) &= H(Ay(t)) \\
&= (H \circ A)(y(t)) \\
&= \tilde{H}(y(t)) \\
&= \tilde{H}(y_0) \\
&= (H \circ A)(y_0) \\
&= H(Ay_0) \\
&= H(AA^+ z_0)
\end{aligned}$$

meaning

$$\Delta H(t) = |H(z_0) - H(AA^+ z_0)|, \quad t \geq 0$$

The greedy method - algorithm

Input: δ, $\Gamma_N = \{\omega_1, \ldots, \omega_N\}$, $\mathbf{z}_0(\omega)$

1. $\omega^* \leftarrow \omega_1$
2. $e_1 \leftarrow \mathbf{z}_0(\omega^*)$
3. $f_1 \leftarrow \mathbb{J}_{2n}^T \mathbf{z}_0(\omega^*)$
4. $A \leftarrow [e_1, f_1]$
5. **while** $\Delta H(\omega) > \delta$ for all $\omega \in \Omega_N$
6. $\quad w^* \leftarrow \operatorname{argmax}_{\omega \in \Omega_N} \Delta H(\omega)$
7. $\quad$ Compute trajectory snapshots $S = \{\mathbf{z}(t_i, \omega^*) | i = 1, \ldots, M\}$
8. $\quad \mathbf{z}^* \leftarrow \operatorname{argmax}_{s \in S} \|s - AA^+ s\|$
9. $\quad$ Apply symplectic Gram-Schmidt on $\mathbf{z}^*$
10. $\quad e_{k+1} \leftarrow \mathbf{z}^* / \|z^*\|$
11. $\quad f_{k+1} \leftarrow \mathbb{J}_{2n}^T \mathbf{z}^*$
12. $\quad A \leftarrow [e_1, \ldots, e_{k+1}, f_1, \ldots, f_{k+1}]$
13. **end while**

The greedy method - convergence

Let S be a subset of $\mathbb{R}^m$ and Y_n, $n \leq m$, be a general n-dimensional subspace of $\mathbb{R}^m$. The Kolmogorov n-width of S in $\mathbb{R}^m$ is given by

$$d_n(S, \mathbb{R}^m) := \inf_{Y_n} \sup_{s \in S} \inf_{y \in Y_n} \|s - y\|_2$$

Theorem

Let S be a compact subset of $\mathbb{R}^{2n}$ with exponentially small Kolmogorov n-width $d_k \leq c \exp(-\alpha k)$ with $\alpha > \log 3$. Then there exists $\beta > 0$ such that the symplectic subspaces A_{2k} generated by the greedy algorithm provide exponential approximation properties such that

$$\|s - P_{2k}(s)\|_2 \leq C \exp(-\beta k)$$

for all $s \in S$ and some $C > 0$.

Hamiltonian reduced model

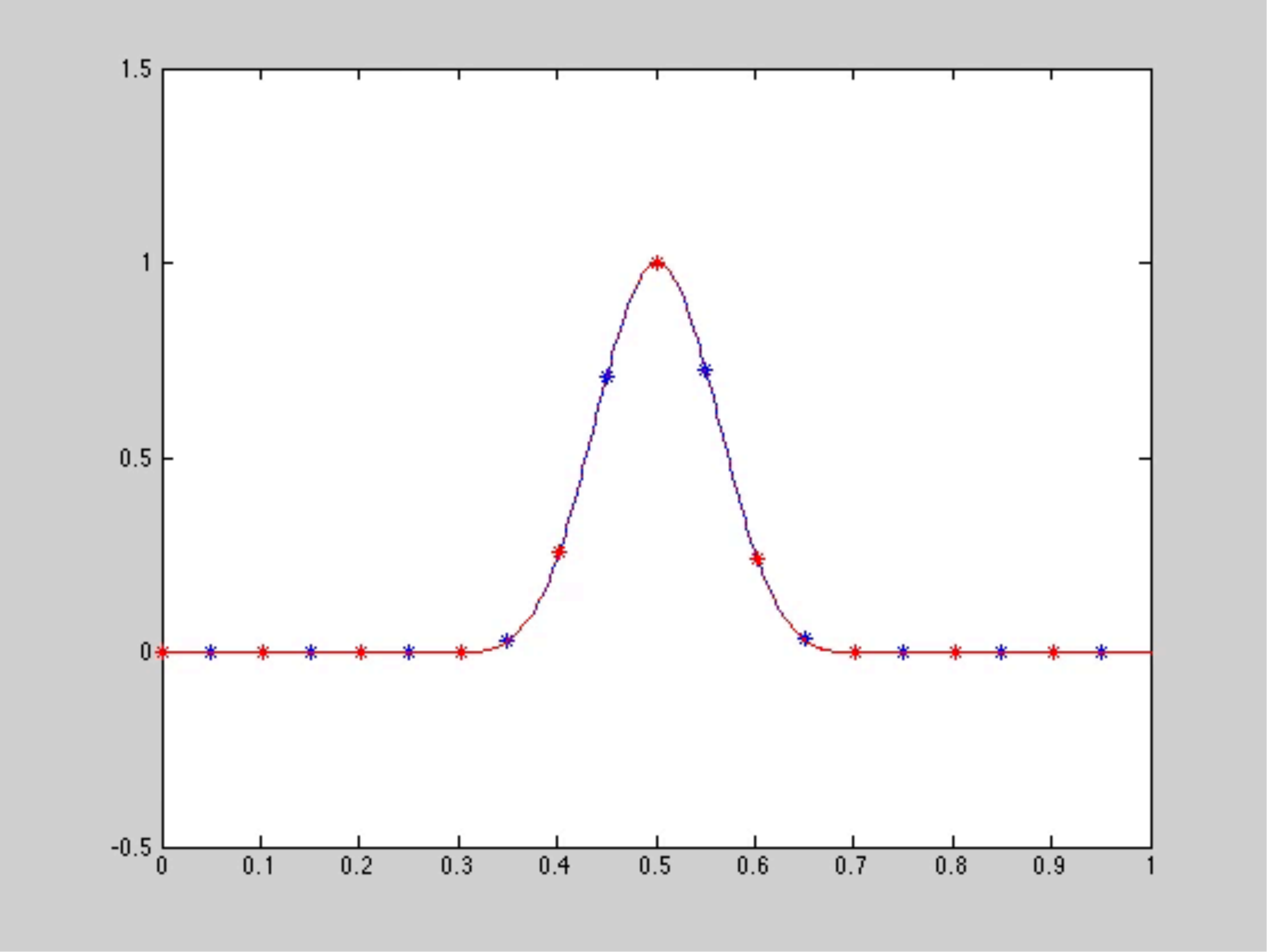
Wave equation:

$$\begin{cases} \dot{q} = p \\ \dot{p} = c^2 q_{xx} \end{cases}$$

Hamiltonian:

$$H(q,p) = \int \left(\frac{1}{2} p^2 + \frac{1}{2} c^2 q_x^2 \right) \, dx$$

- size of original system : 1000
- size of reduced system : 30
- $\Delta H = 5 \times 10^{-4}$.
- $||y - y_r||_{L_2} = 5 \times 10^{-5}$



Stability by construction

Hamiltonian reduced model

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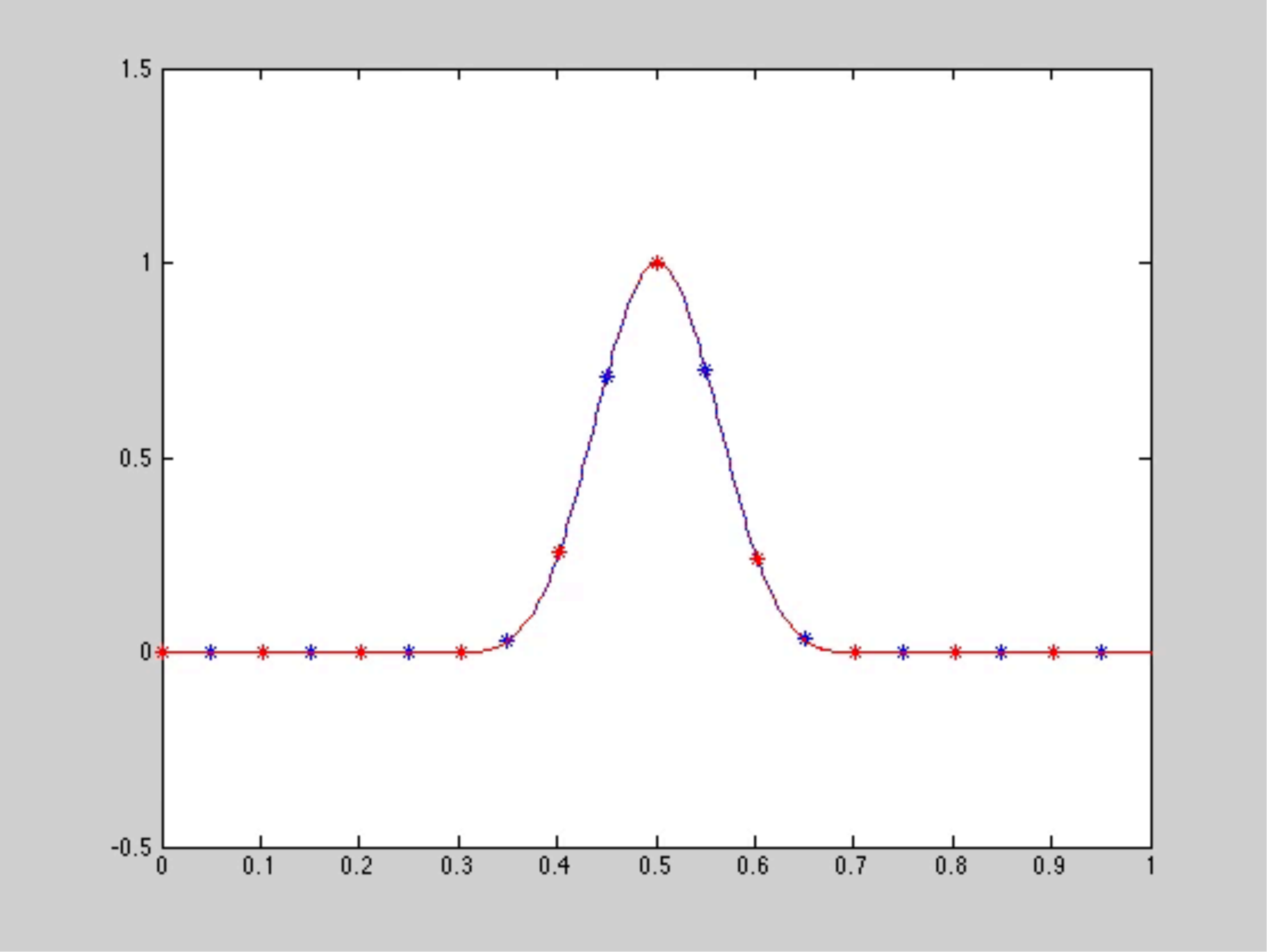

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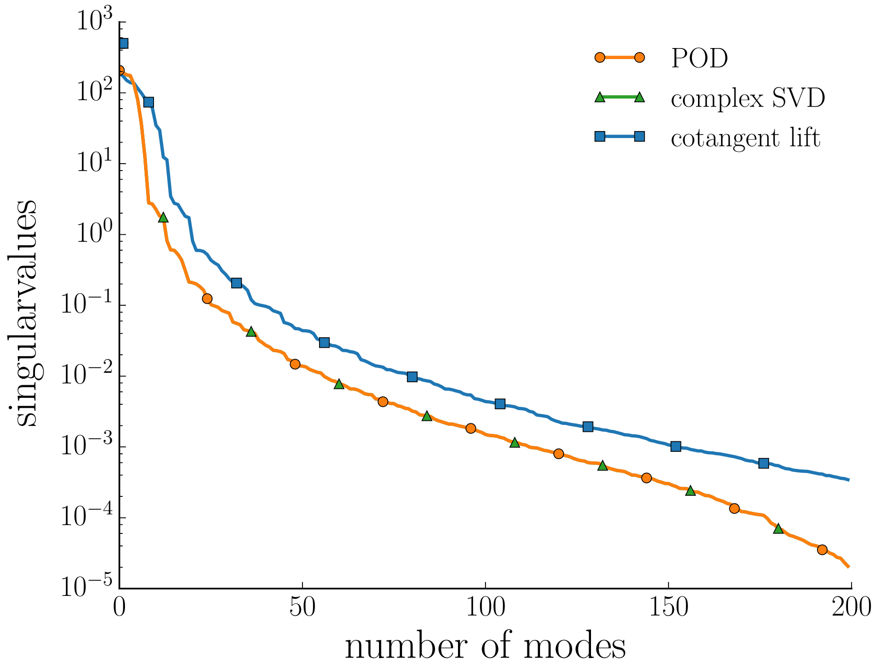
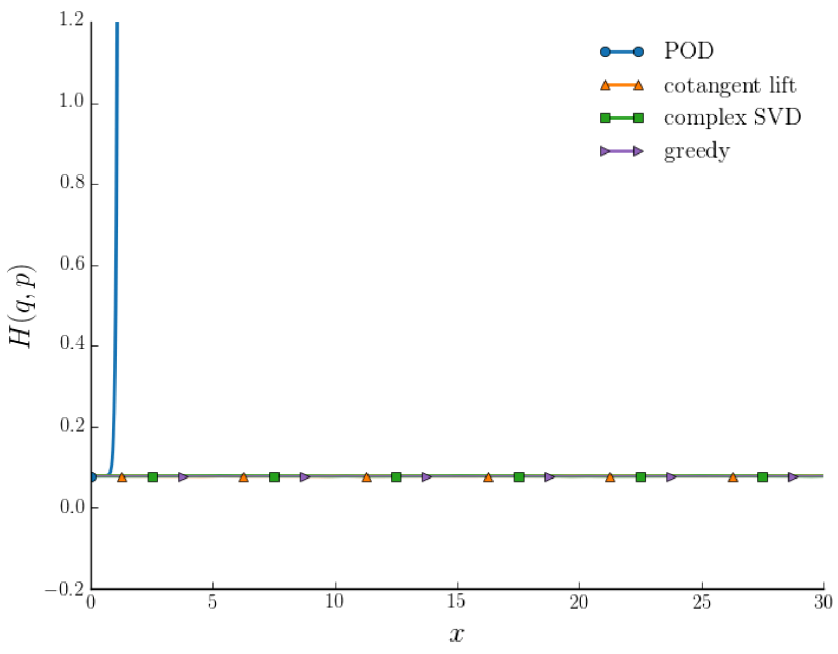
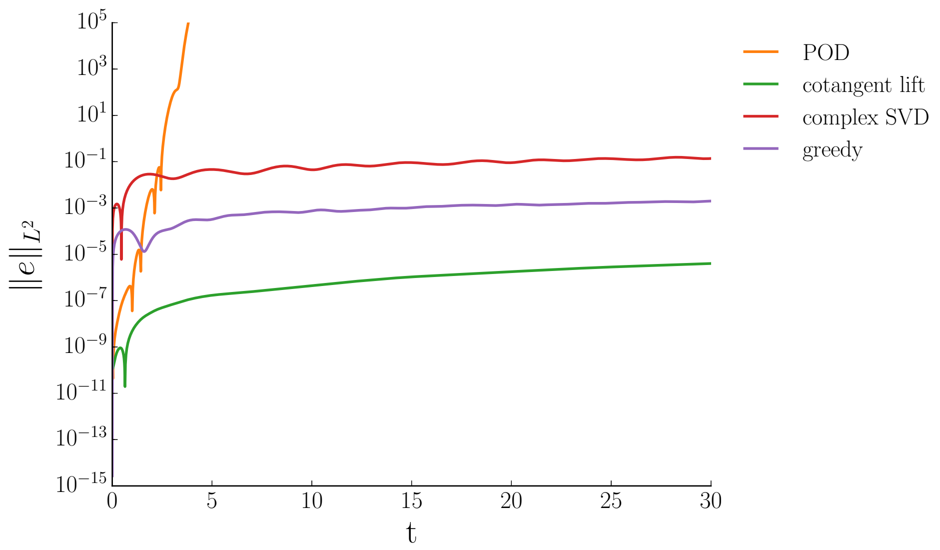


(d)



(e)



(f)

Symplectic Empirical Interpolation

Nonlinear case:

$$\frac{d}{dt}\mathbf{z} = L\mathbf{z} + \mathbf{g}(z) \Longrightarrow \frac{d}{dt}\mathbf{y} = \tilde{L} + A^{+}\mathbf{g}(A\mathbf{y})$$

Let $H = H_1 + H_2$ such that $\nabla_z H_1 = L$ and $\nabla_z H_2 = g$. The (D)EIM approximation then is

$$\frac{d}{dt}\mathbf{y} = \tilde{L}\mathbf{y} + \underbrace{A^{+}\mathbb{J}_{2n}U(P^TU)^{-1}P^T\mathbf{g}(A\mathbf{y})}_{\tilde{N}(\mathbf{y})}$$

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This system is a Hamiltonian system if and only if

$$\tilde{N}(\mathbf{y}) = \mathbb{J}_{2k}\nabla_{\mathbf{y}}h(\mathbf{y})$$

Note that $g = \nabla_z H_2 = (A^{+})^T \nabla_y H_2$. And if we take $U = (A^{+})^T$

$$\tilde{N}(\mathbf{y}) = A^{+}\mathbb{J}_{2n}(A^{+})^T(P^T(A^{+})^T)^{-1}P^T(A^{+})^T\nabla_y H_2 = \mathbb{J}_{2k}\nabla_y H_2(A\mathbf{y})$$

Schrödinger's equation

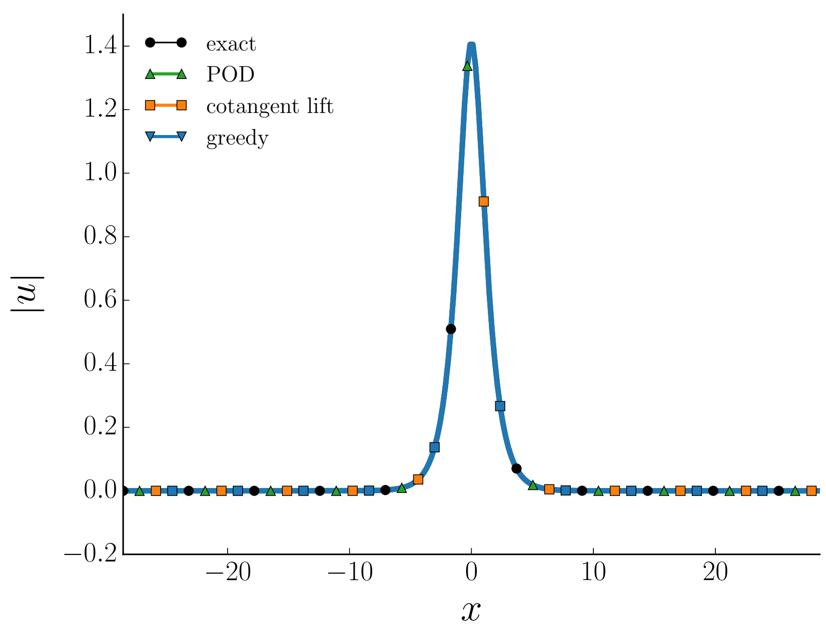
Schrödinger Equation

$$\begin{cases} q_t = p_{xx} + \epsilon(q^2 + p^2)p, \\ p_t = -q_{xx} - \epsilon(q^2 + p^2)q, \end{cases}$$

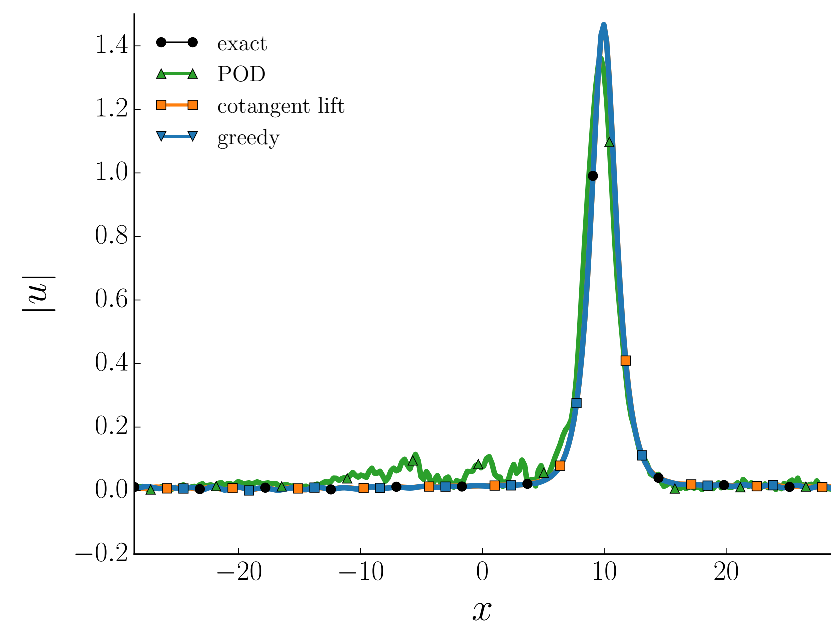
With discrete Hamiltonian:

$$H_{\Delta x}(\mathbf{z}) = \Delta x \sum_{i=1}^{N} \left(\frac{q_i q_{i-1} - q_i^2}{\Delta x^2} + \frac{p_i p_{i-1} - p_i^2}{\Delta x^2} + \frac{\epsilon}{4}(p_i^2 + q_i^2)^2 \right)$$

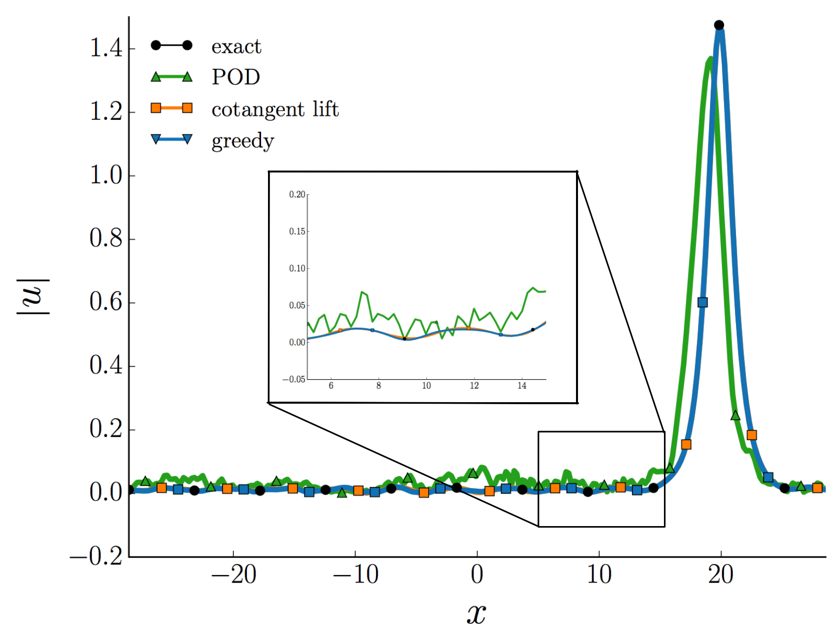
Schrödinger's equation



(g) $t = 0$



(h) $t = 10$



(i) $t = 20$

Shallow water equations

Let us return to the shallow water equation

$$\begin{cases} h_t + \nabla \cdot (h \nabla \phi) = 0 \\ \phi_t + \frac{1}{2}|\nabla \phi|^2 + h = 0 \end{cases} \qquad \mathbf{u} = \nabla \phi$$

With the Hamiltonian

$$H(p,q) = \frac{1}{2} \int h^2 + h|\nabla \phi|^2 \, dx$$

$$h_t = \frac{\delta H}{\delta \phi}, \qquad \phi_t = \frac{\delta H}{\delta h},$$

Hence, we can use the same machinery to solve SWE

Shallow water equations

Solved as

- Fourier spectral method in space
- Filtering for stability
- Symplectic time integration

$$
\begin{aligned}
p^{n+\frac{1}{2}} &= p^n - \frac{h}{2}\frac{\delta H}{\delta q}(p^{n+\frac{1}{2}}, q^n),\\
q^{n+1} &= q^n + \frac{h}{2}\left(\frac{\delta H}{\delta p}(p^{n+\frac{1}{2}}, q^n) + \frac{\delta H}{\delta p}(p^{n+\frac{1}{2}}, q^{n+1})\right),\\
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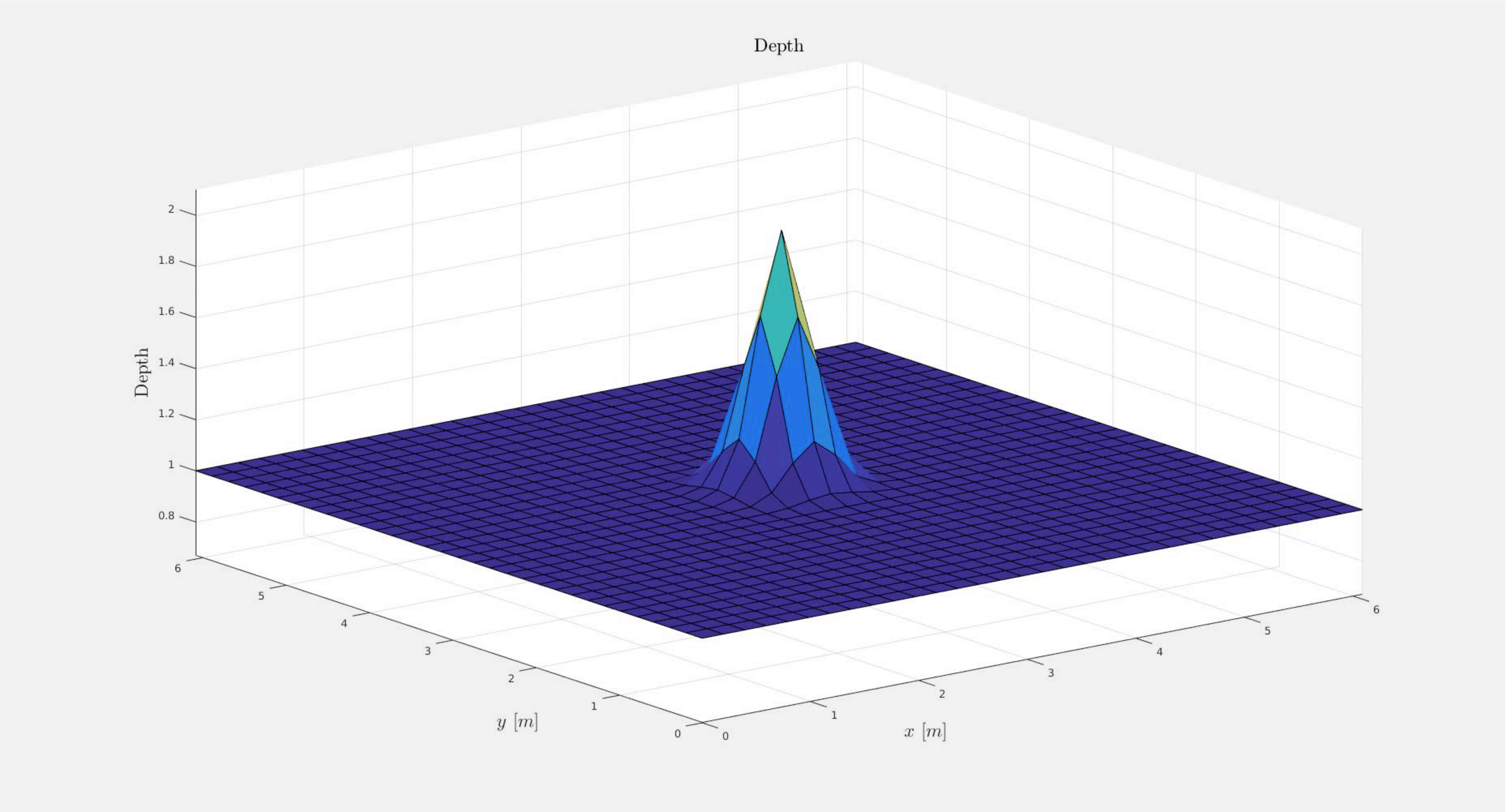
$$p^{n+1} = p^n - \frac{h}{2}\frac{\delta H}{\delta q}(p^{n+\frac{1}{2}}, q^{n+1}),$$

For reduced model

- POD using RK4 since symplectic structure is lost
- Symplectic ROM integrated same way

Shallow water equations

POD - k=80



Shallow water equations

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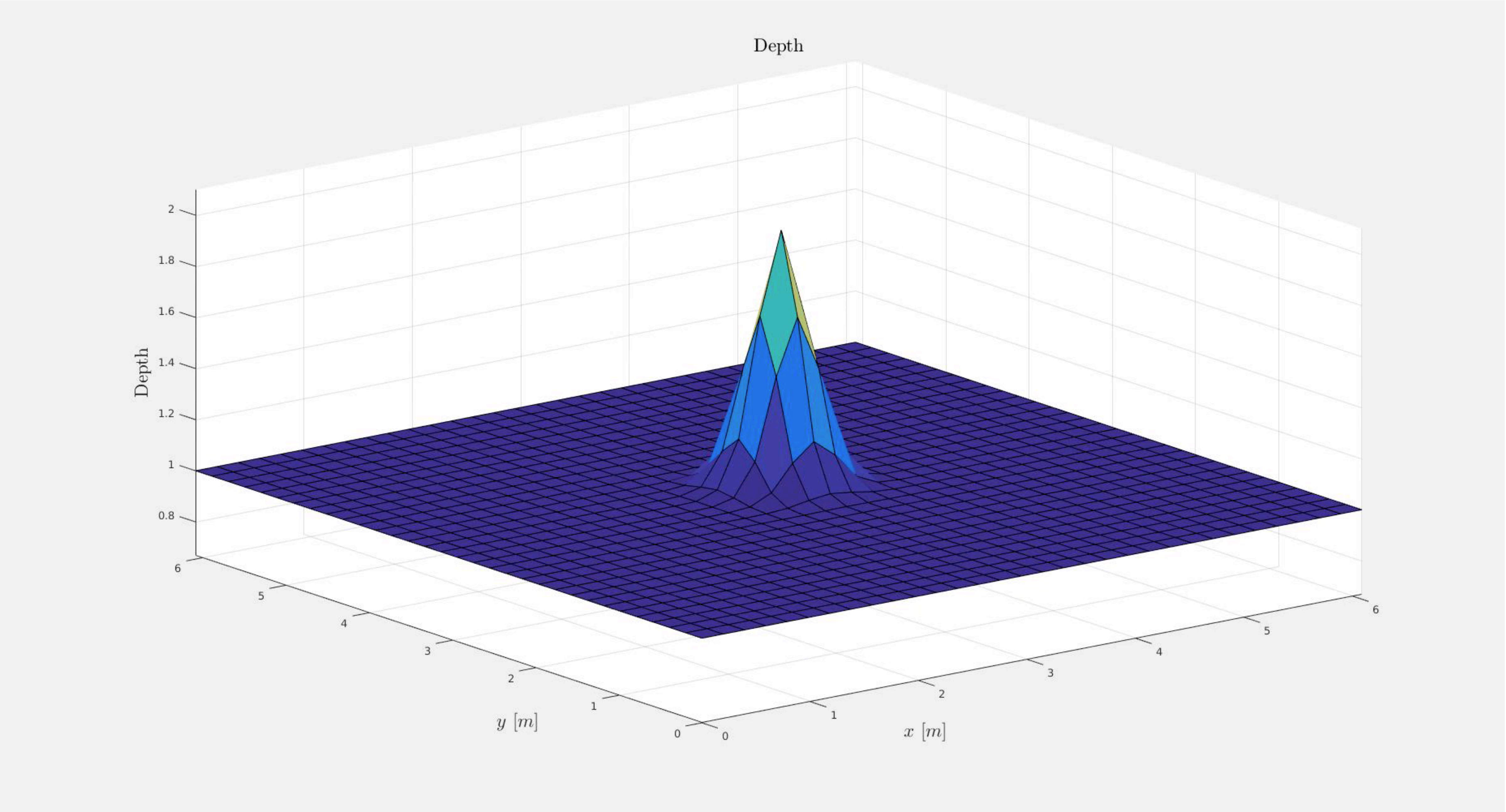
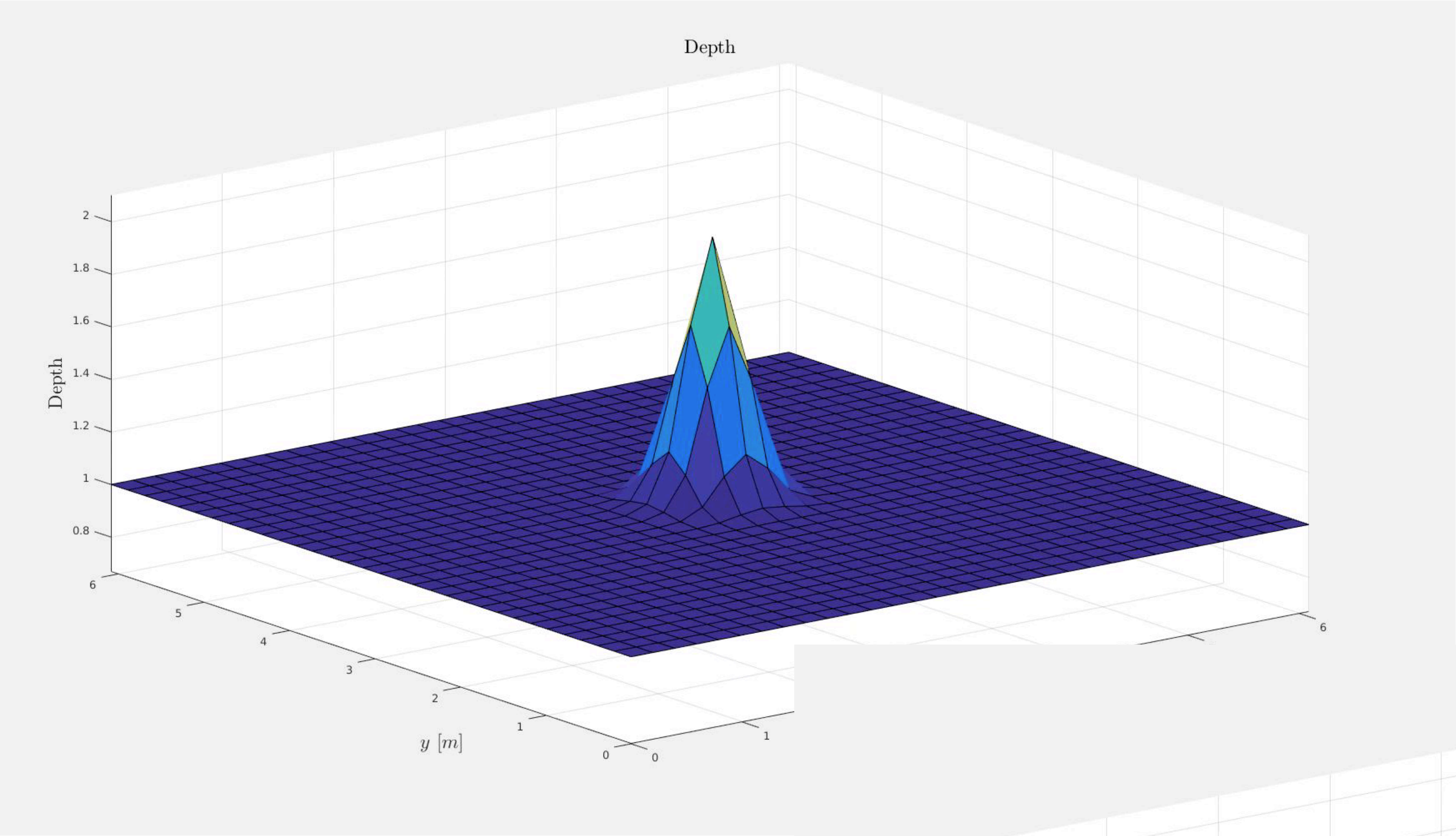
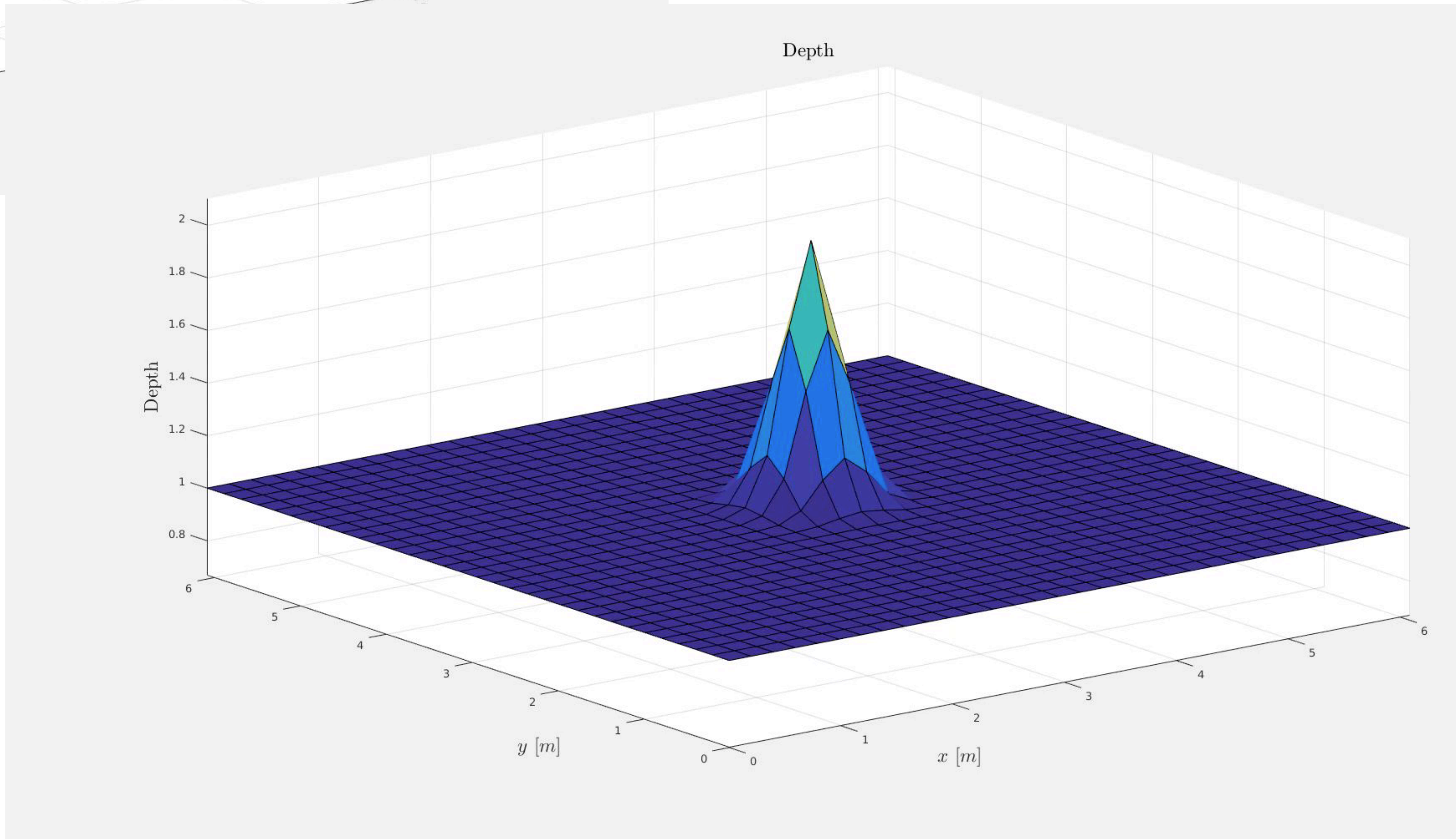


Shallow water equations





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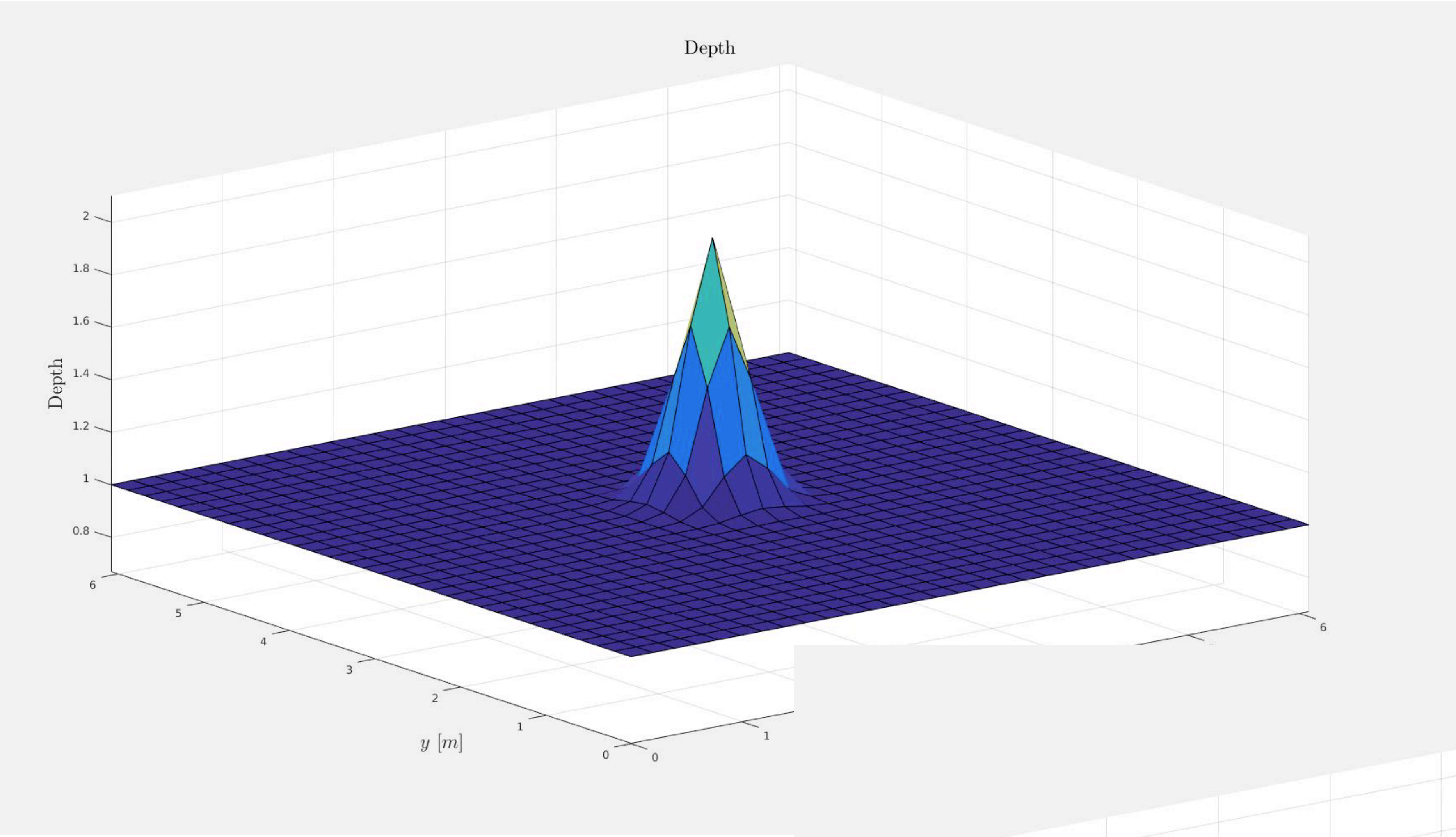
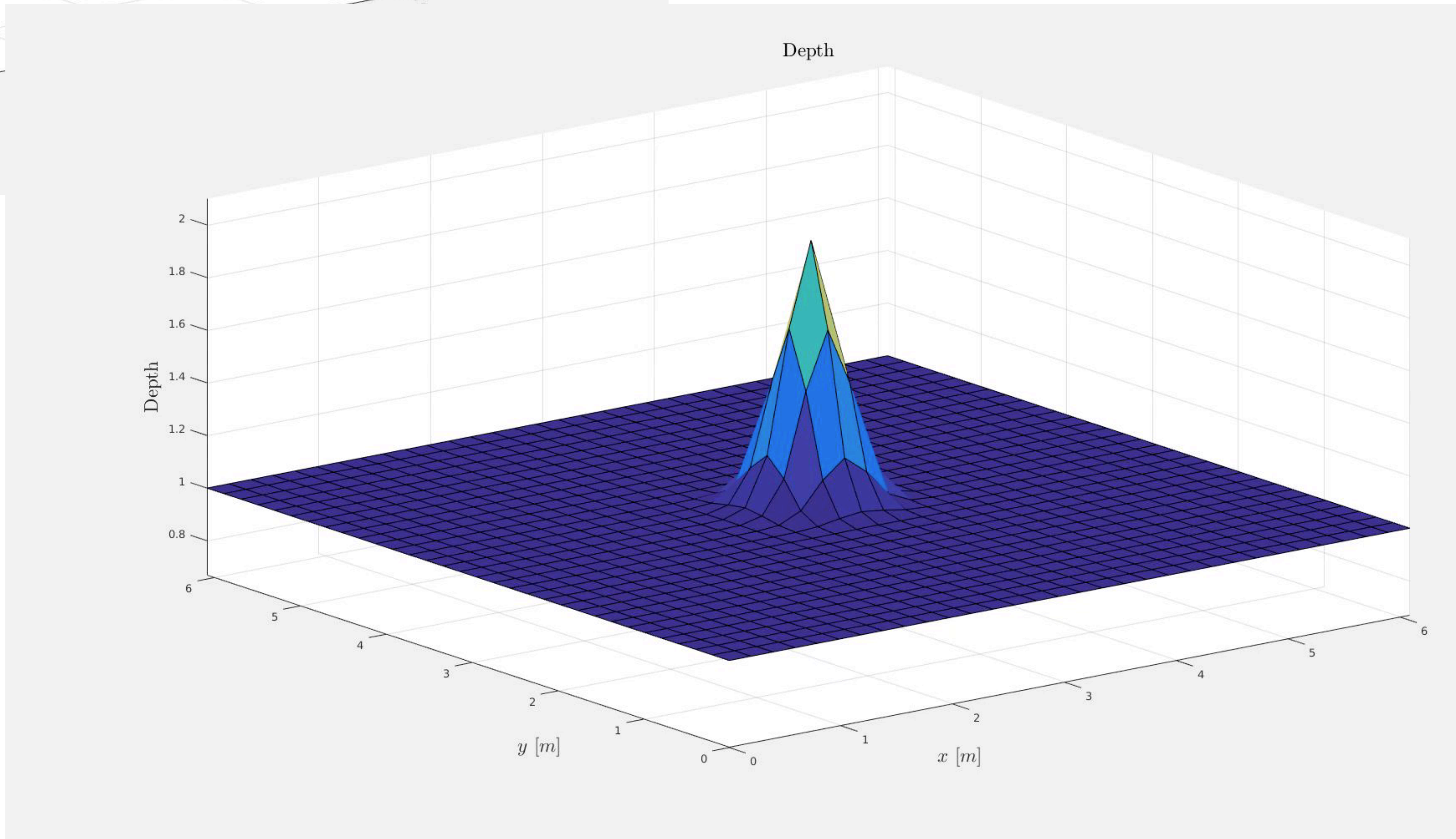
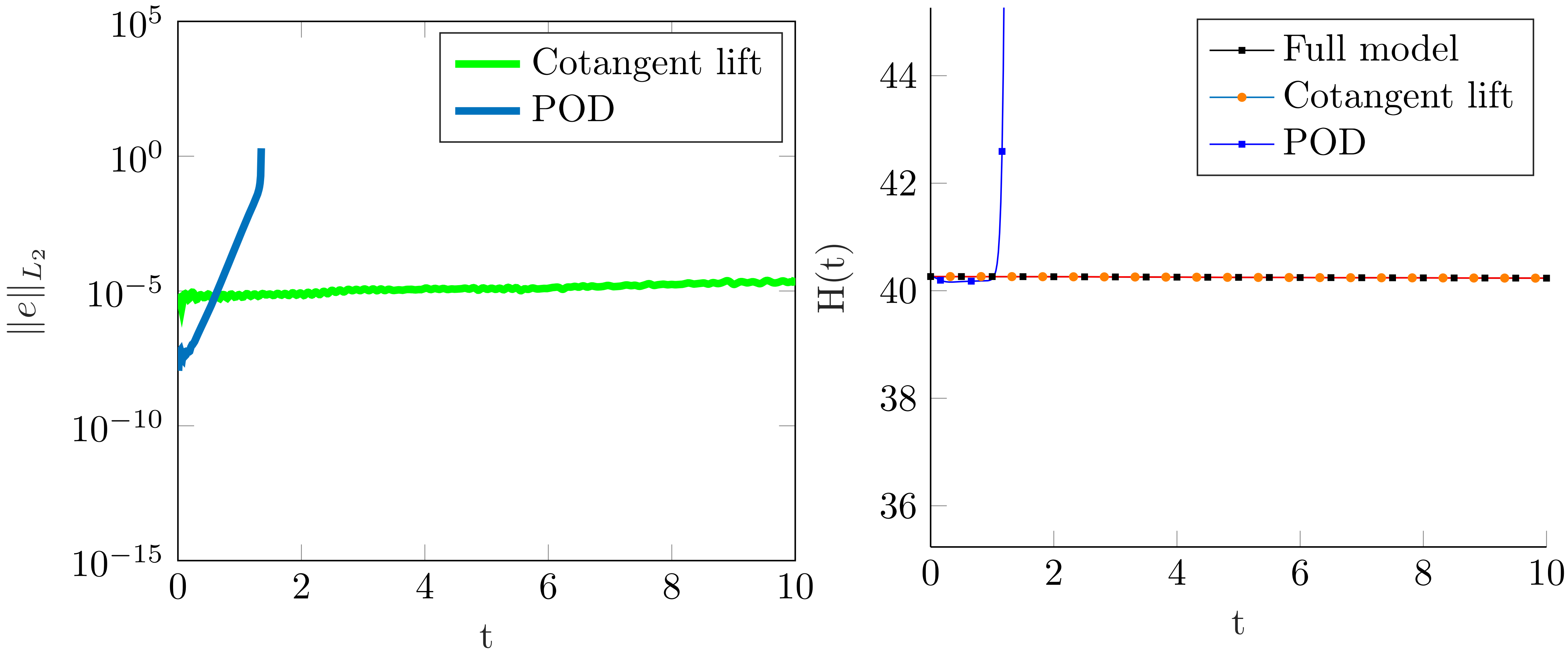


Full model - n=1024



Reduced model
k=80

Shallow water equations



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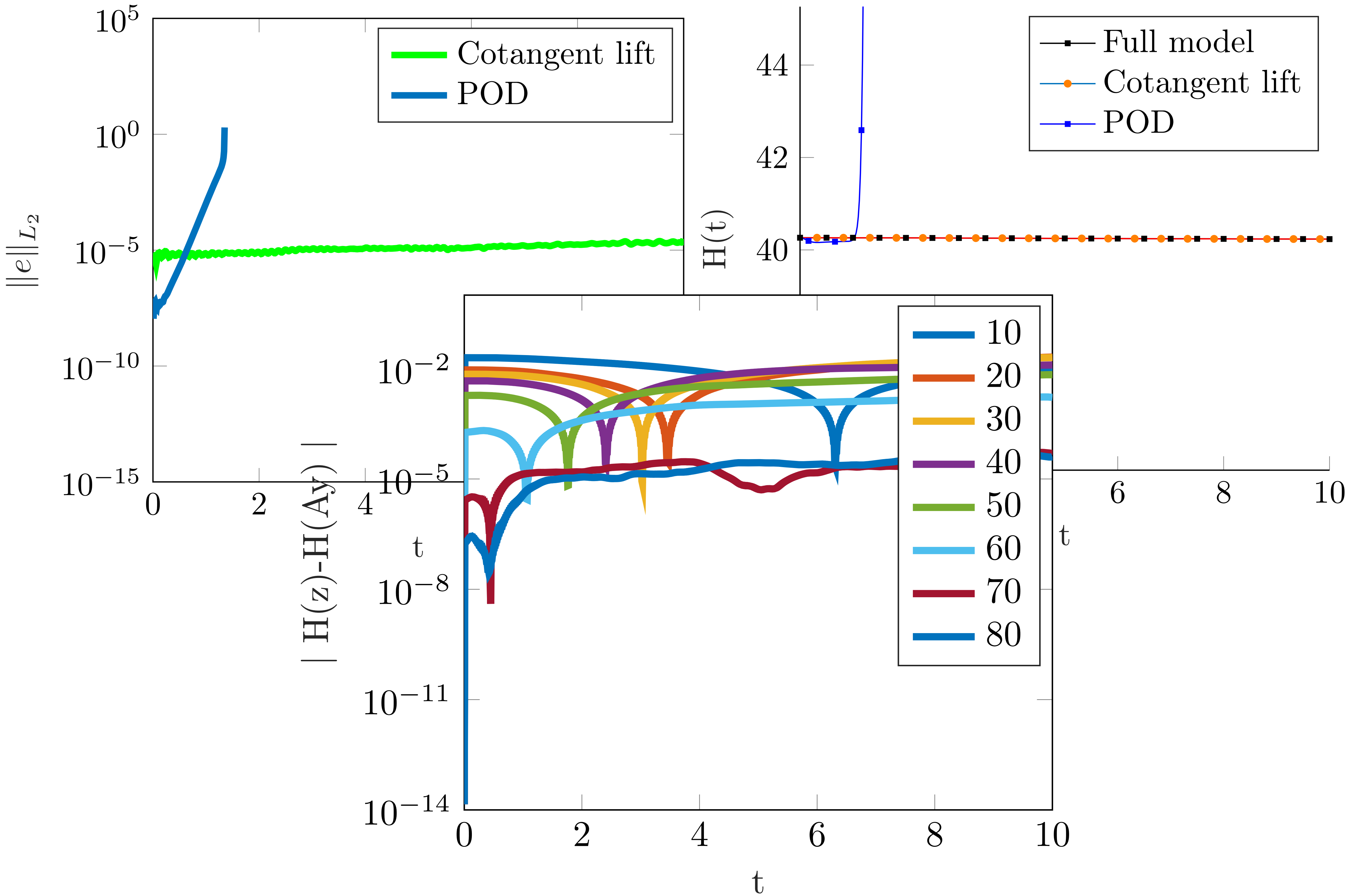

Beyond Hamiltonian systems

Let us consider a more general problem with dissipation in which case the simple Hamiltonian structure vanishes

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Existing model reduction techniques:

- Integrating a non-conservative system $\Rightarrow$ accumulation of local error on long-time Integration
- Integrating a non-conservative system with a symplectic integrator $\Rightarrow$ no guarantee of energy conservation

Beyond Hamiltonian systems

Let us consider a more general problem with dissipation in which case the simple Hamiltonian structure vanishes

Existing model reduction techniques:

- Integrating a non-conservative system $\Rightarrow$ accumulation of local error on long-time Integration
- Integrating a non-conservative system with a symplectic integrator $\Rightarrow$ no guarantee of energy conservation

We shall consider an alternative

Beyond Hamiltonian systems

We consider a more general problem

$$\dot{z} = \mathbb{J}_{2n} K^T K z - R z,$$

We express the system as

$$\dot{z} = \mathbb{J}_{2n} K^T f(t), \qquad f(t) + \int_0^t \chi(t-s) \cdot f(s)\, ds = Kz$$

$$\chi \geq 0$$

Often called the time-dissipative-dispersive model (TDD)

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Often called the time-dissipative-dispersive model (TDD)

If susceptibility is zero, original Hamiltonian problem recovered

Hence, the Volterra integral accounts for history effects

Beyond Hamiltonian systems

A TDD Hamiltonian system can be extended to a closed one (Figotin et al, 2006)

$$\begin{cases} \dot{z} = \mathbb{J}_{2n} K^T f(t) \\ \phi_t(t,x) = \theta(t,x) \\ \theta_t(t,x) = \phi_{xx}(t,x) + \sqrt{2}\delta_0(x)\sqrt{\chi} f(t) \end{cases}$$

with the expression $f(t) + \sqrt{2}\sqrt{\chi}\phi(t,0) = Kz(t)$

and the extended Hamiltonian

$$H_{\text{ex}}(z,\phi,\theta) = \frac{1}{2}\left(\|Kz - \phi(t,0)\|_2^2 + \|\theta(t)\|_{\mathcal{H}^{2n}}^2 + \|\partial_x \phi(t)\|_{\mathcal{H}^{2n}}^2\right)$$

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Strings carry the dissipation

Beyond Hamiltonian systems

Given a symplectic basis A:

$$z = Ay,\ \tilde{f} = Af,\ \tilde{\phi} = A\phi,\ \tilde{\theta} = A\theta$$

The RDH system reads

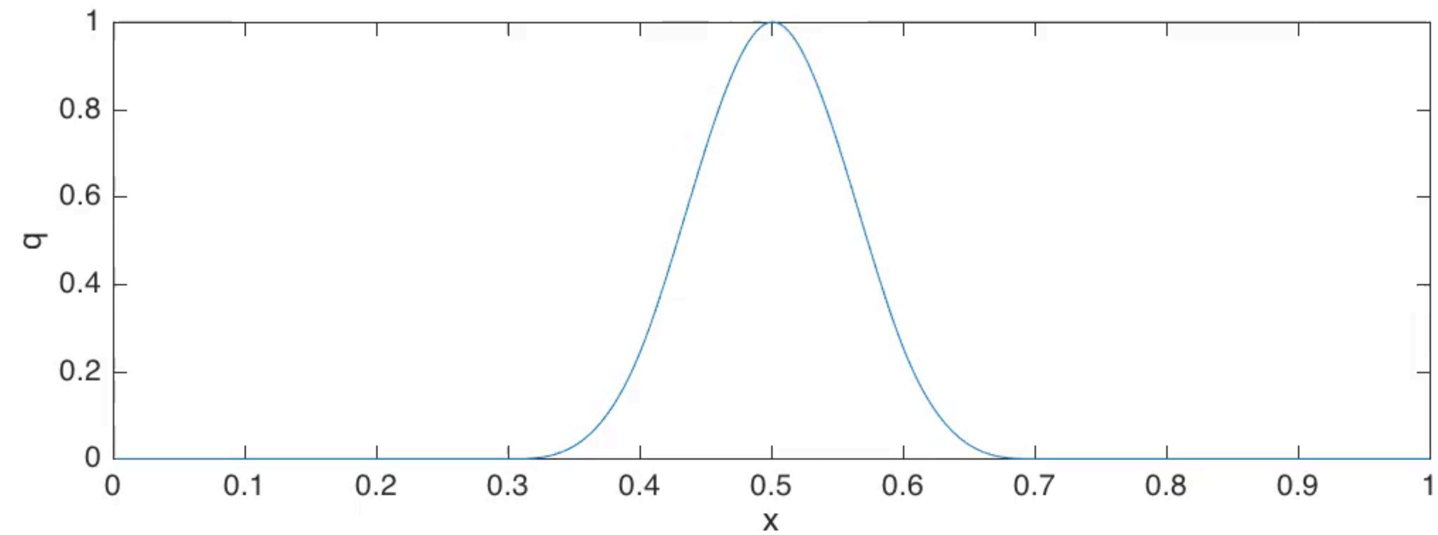
$$\begin{aligned}
&\dot{y}(t) = \mathbb{J}_{2k}\tilde{L}^T\tilde{f}(t)\\
&\partial_t\tilde{\phi}(t,x) = \tilde{\theta}(t,x)\\
&\partial_t\tilde{\theta}(t,x) = \partial_x^2\tilde{\phi}(t,x) + \sqrt{2}\delta_0(x)\cdot\sqrt{\tilde{\chi}}\tilde{f}(t)
\end{aligned}$$

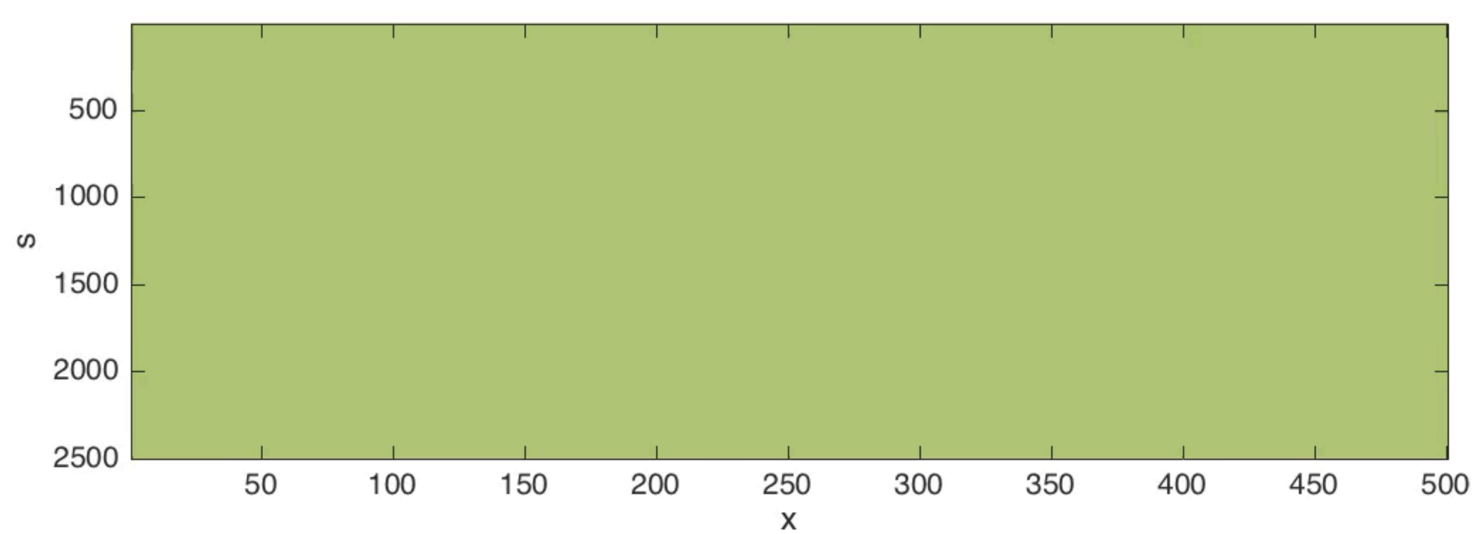
Where $\tilde{L} = A^TLA$ and $K^TK = L^TL$.

Beyond Hamiltonian systems

Consider first the damped wave equation

$$\begin{cases} q_t(t,x) = p(t,x), \\ p_t(t,x) = c^2 q_{xx}(t,x) - r(x)p(t,x), \\ q(0,x) = q_0(x), \\ p(0,x) = 0. \end{cases}$$





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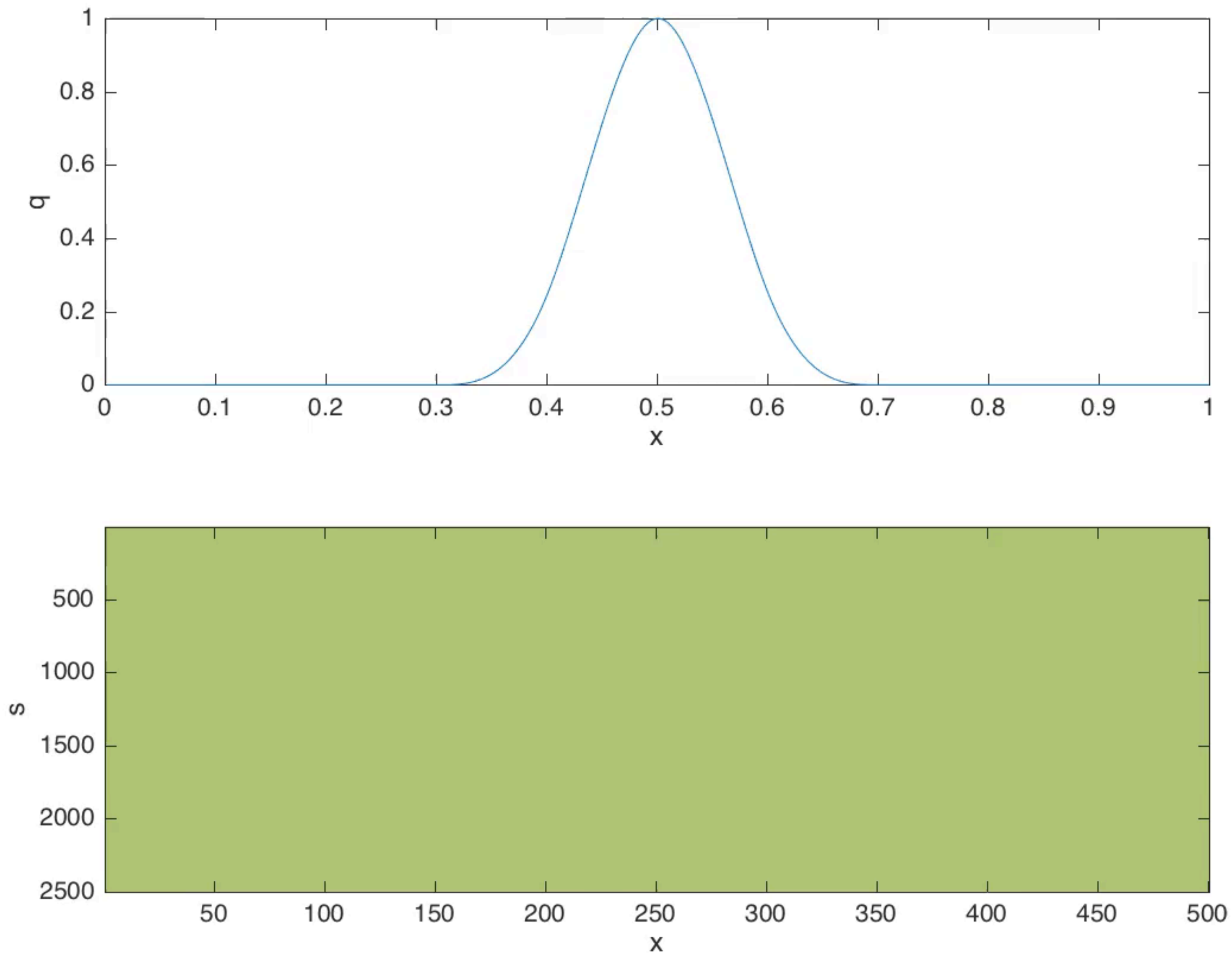
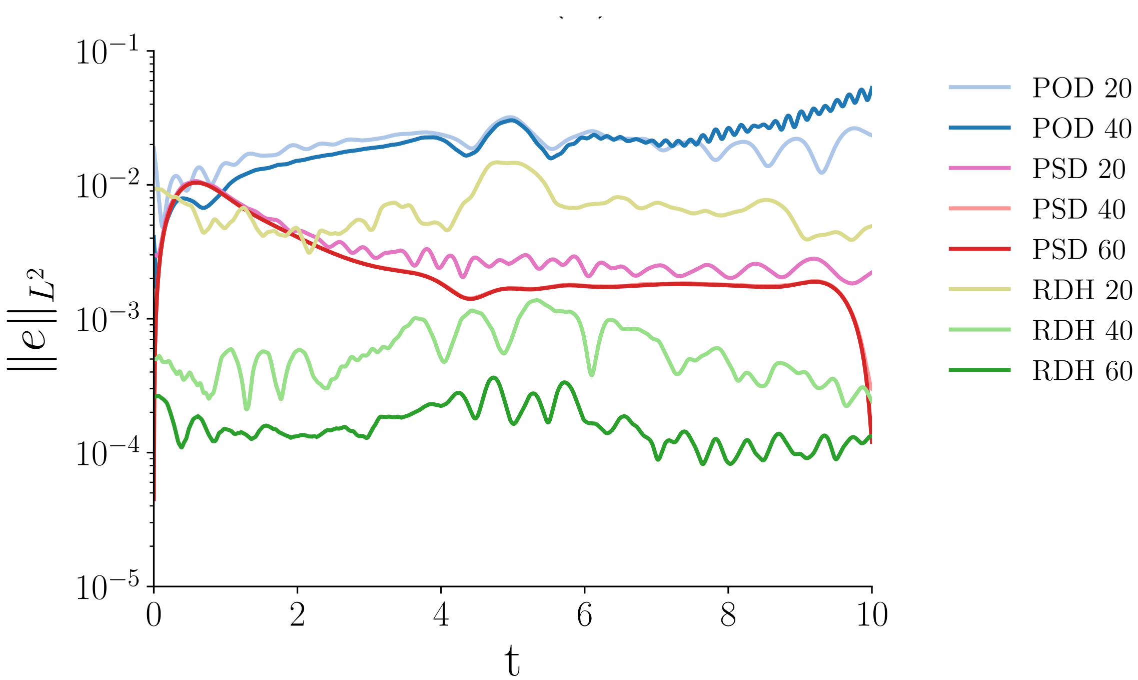
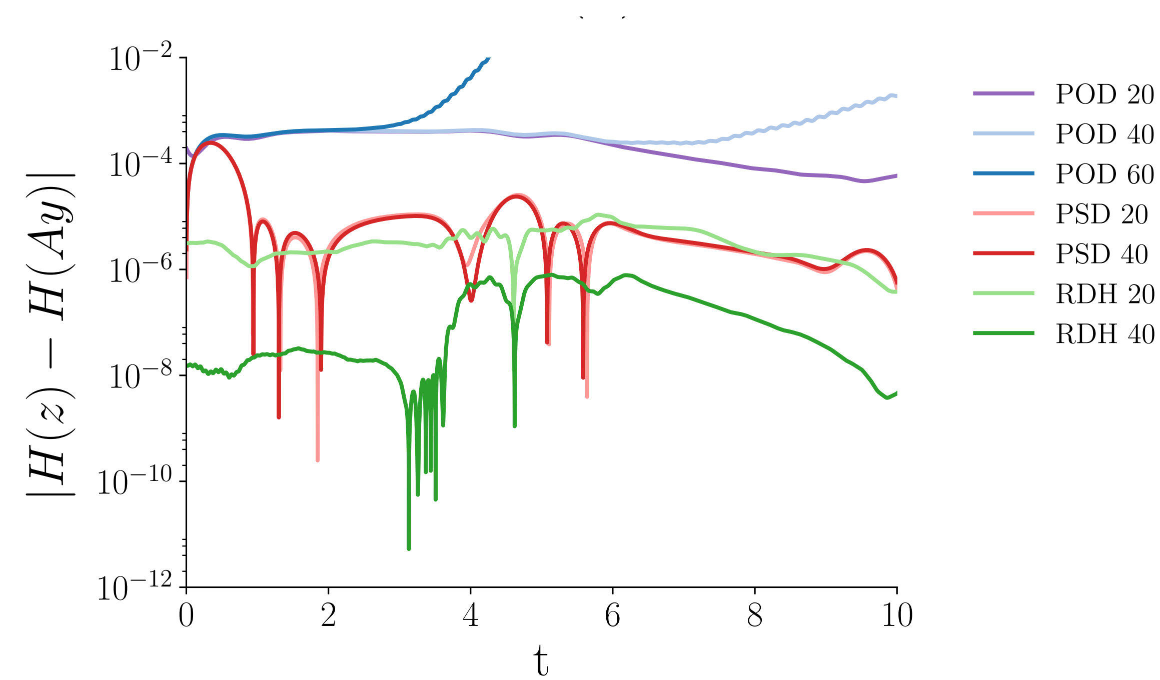
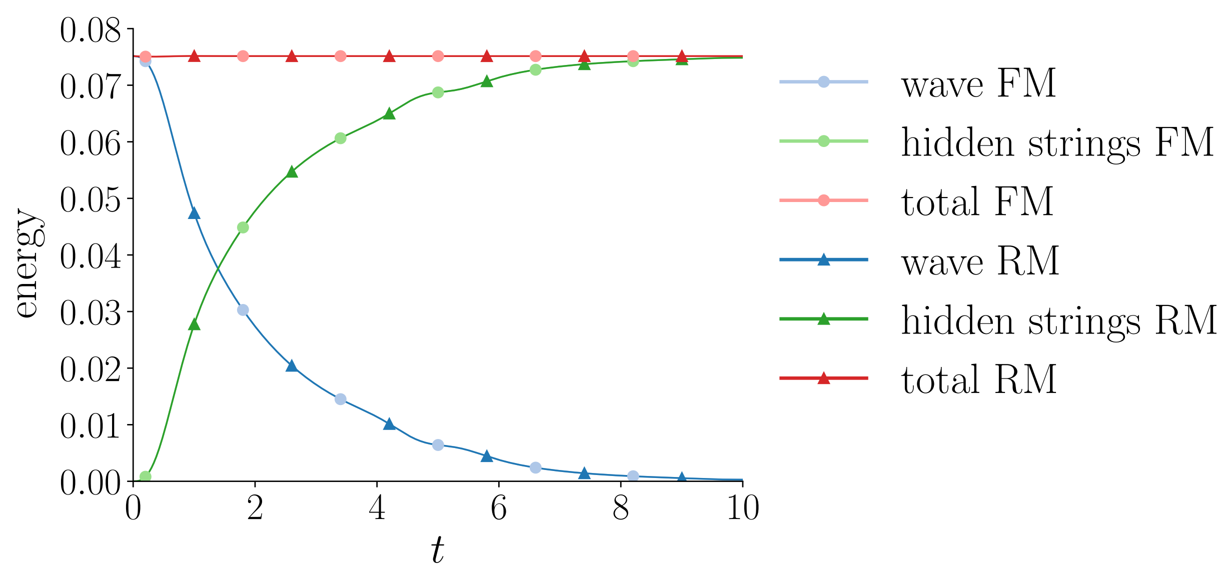
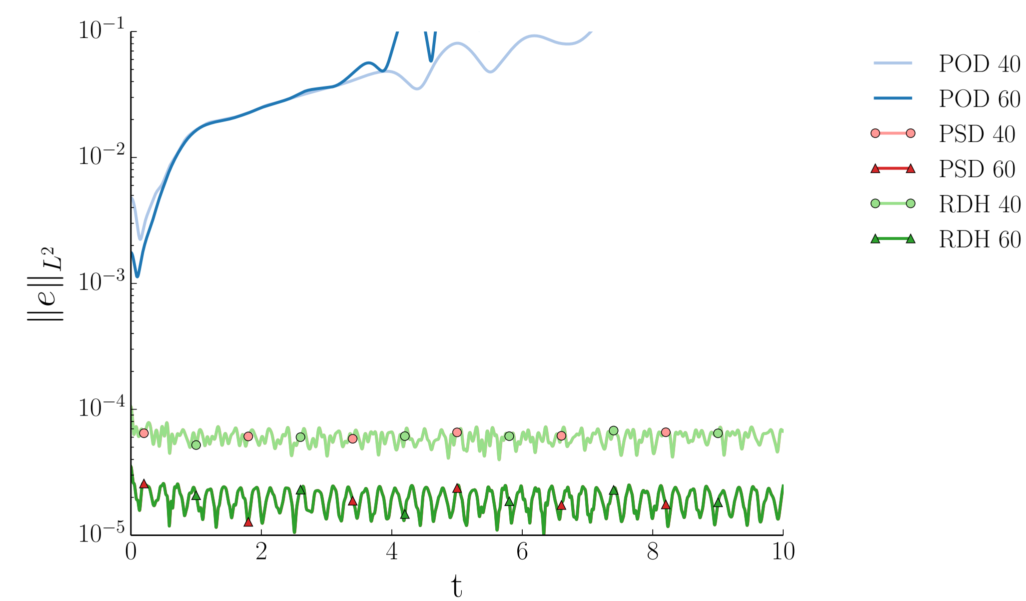


Beyond Hamiltonian systems





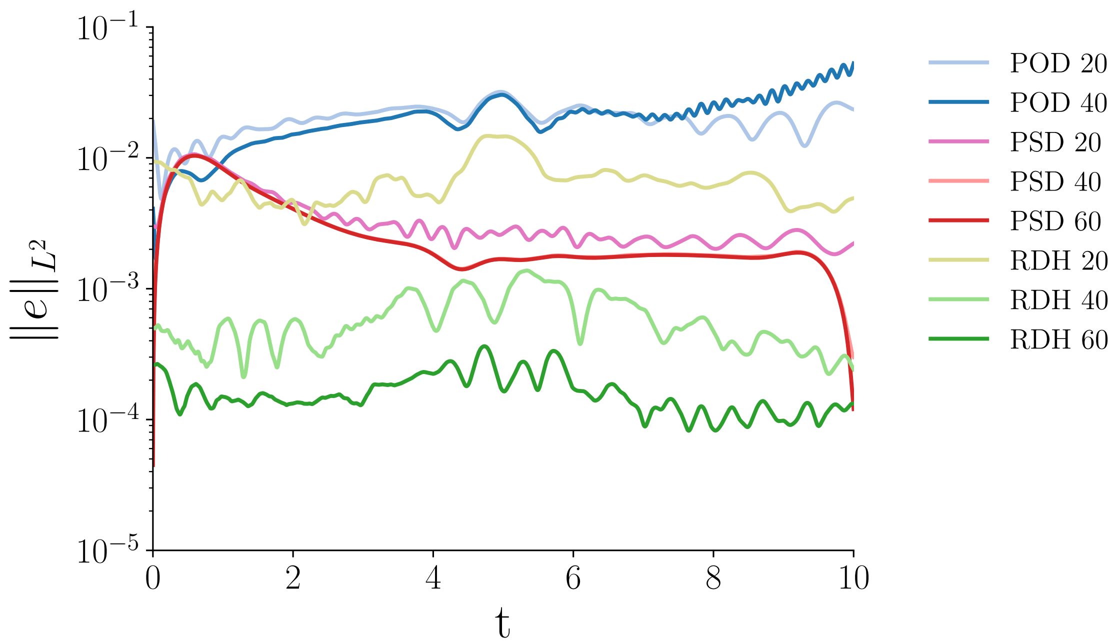




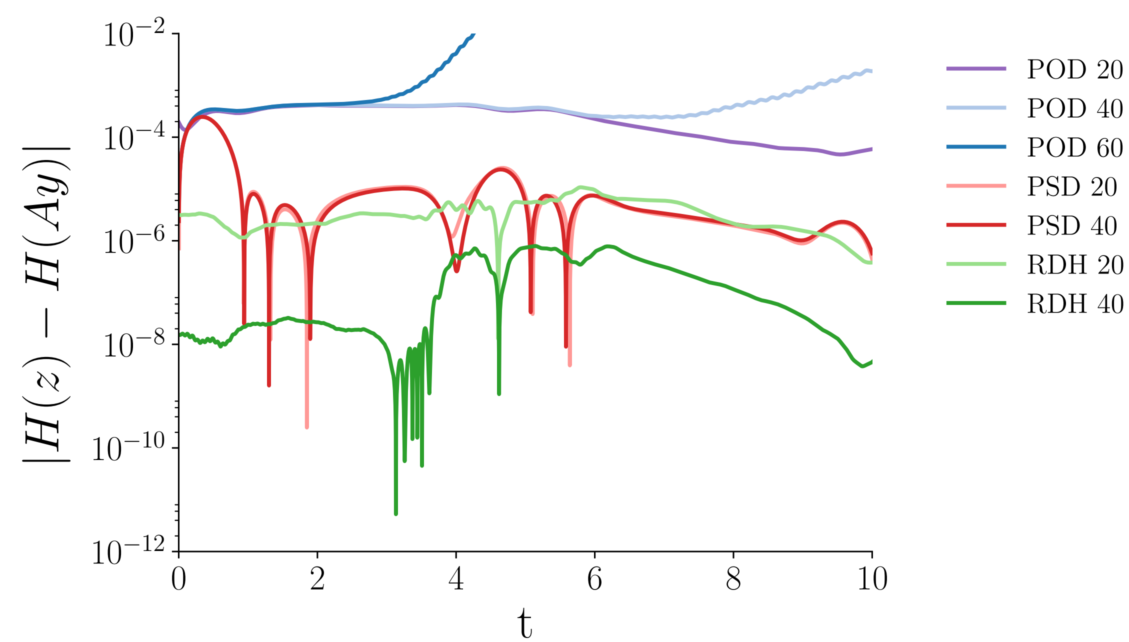
Beyond Hamiltonian systems

Extension to non-linear Sine-Gordon equation

$$q_t = p,$$
$$p_t = q_{xx} - \sin(q) - r(x)p,$$

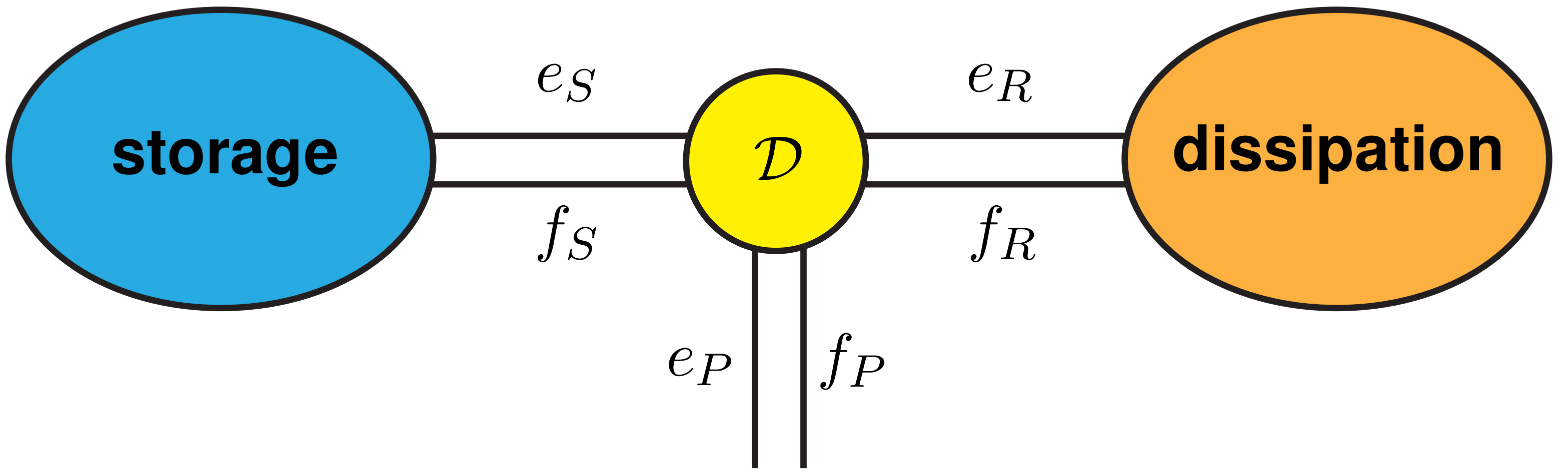


error



conservation of energy

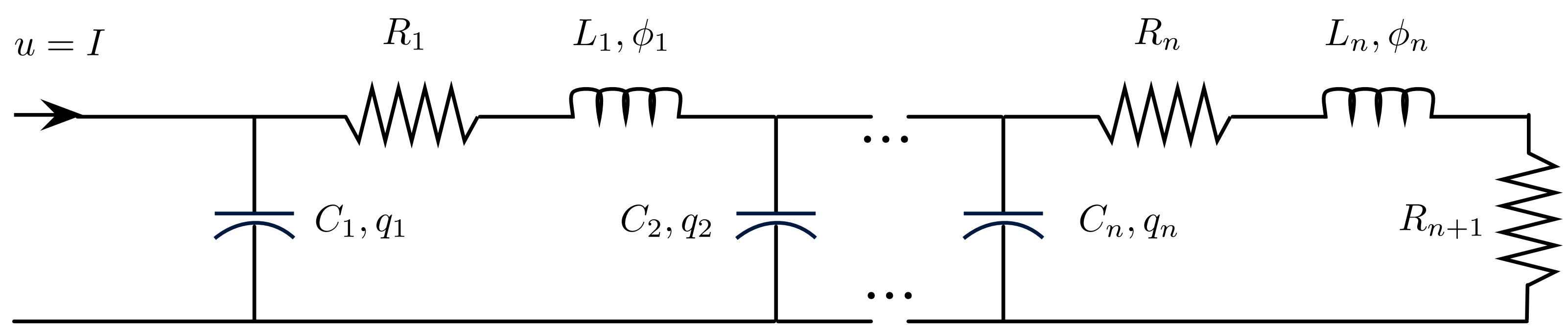
Beyond Hamiltonian systems



Linear port-Hamiltonian systems

$$\dot{x} = (J_{2n} - R)Q^T Q x + u$$

Beyond Hamiltonian systems



We have

$$Q = \text{diag}(C_1^{-1}, L_1^{-1}, \ldots, C_n^{-n}, L_n^{-n})$$

$$R = \text{diag}(0, R_1, \ldots, 0, R_n + R_{n+1})$$

$$J_{2n} = \begin{pmatrix} 0 & 1 & 0 & \\ -1 & 0 & 1 & \\ 0 & -1 & 0 & \\ & & & \ddots \end{pmatrix}$$

Give rise to the port Hamiltonian system

$$\dot{x} = (J_{2n} - R)Q^T Qx + u$$

Beyond Hamiltonian systems

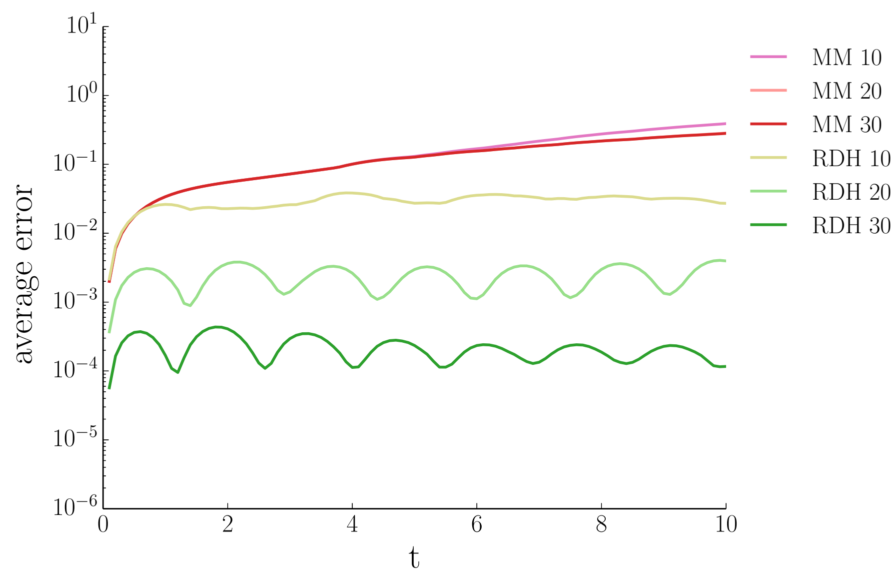
With a change of coordinate/variables we re-write as a dissipative Hamiltonian system:

$$\dot{\tilde{x}} = \mathbb{J}_{2n}\tilde{Q}^T\tilde{Q}\tilde{x} - \tilde{R}x + \tilde{u}$$

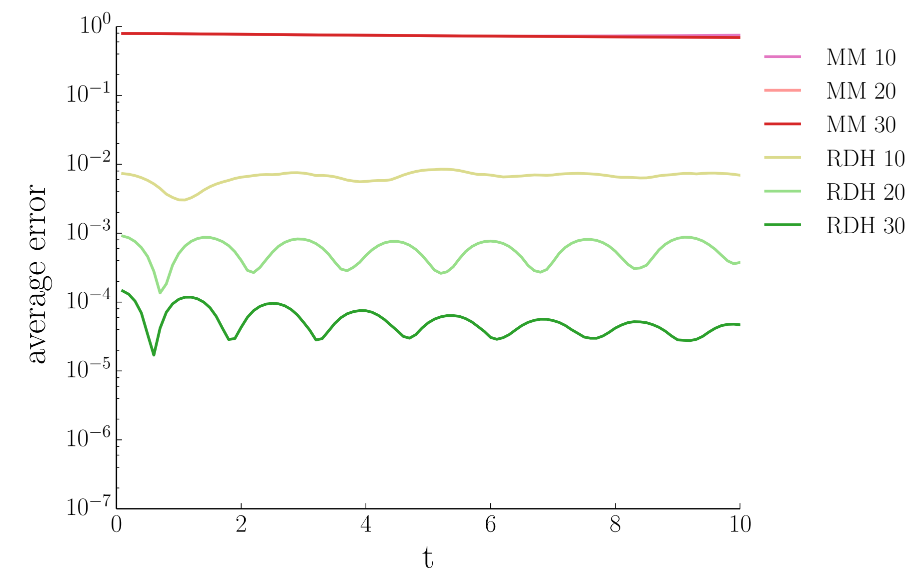
which corresponds to the TDD system

$$\dot{\tilde{x}} = \mathbb{J}_{2n}\tilde{Q}^T f(t) + \tilde{u}, \quad f(t) + \tilde{R}\int_0^t f(t) = \tilde{Q}\tilde{x}.$$

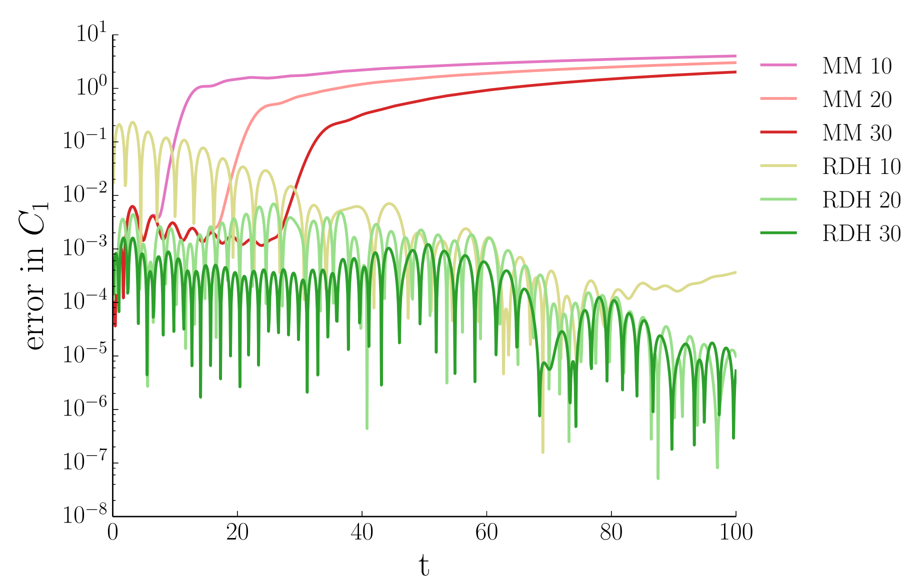
Beyond Hamiltonian systems



(a) capacitors



(b) inductors



(c) charge in C_1

Euler/Navier-Stokes equations

Let us finally consider the Euler/Navier-Stokes equations

$$\partial_t u_\alpha + \partial_{x_\beta} u_\beta u_\alpha + \partial_{x_\alpha} p = \nu \Delta u_\alpha$$

$$\partial_{x_\alpha} u_\alpha = 0$$

Developing a ROM directly for this is unstable

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Developing a ROM directly for this is unstable

There is a generalized Hamiltonian structure for the Euler equations - but it is complicated

We use the skew-symmetric form

$$\partial_t u_\alpha + \frac{1}{2}\left(\partial_{x_\beta} u_\beta u_\alpha + u_\beta \partial_{x_\beta} u_\alpha\right) + \partial_{x_\alpha} p = \nu \Delta u_\alpha$$

This conserves energy - also at discrete level

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$$\partial_{x_\alpha} u_$$

Developing a ROM directly for

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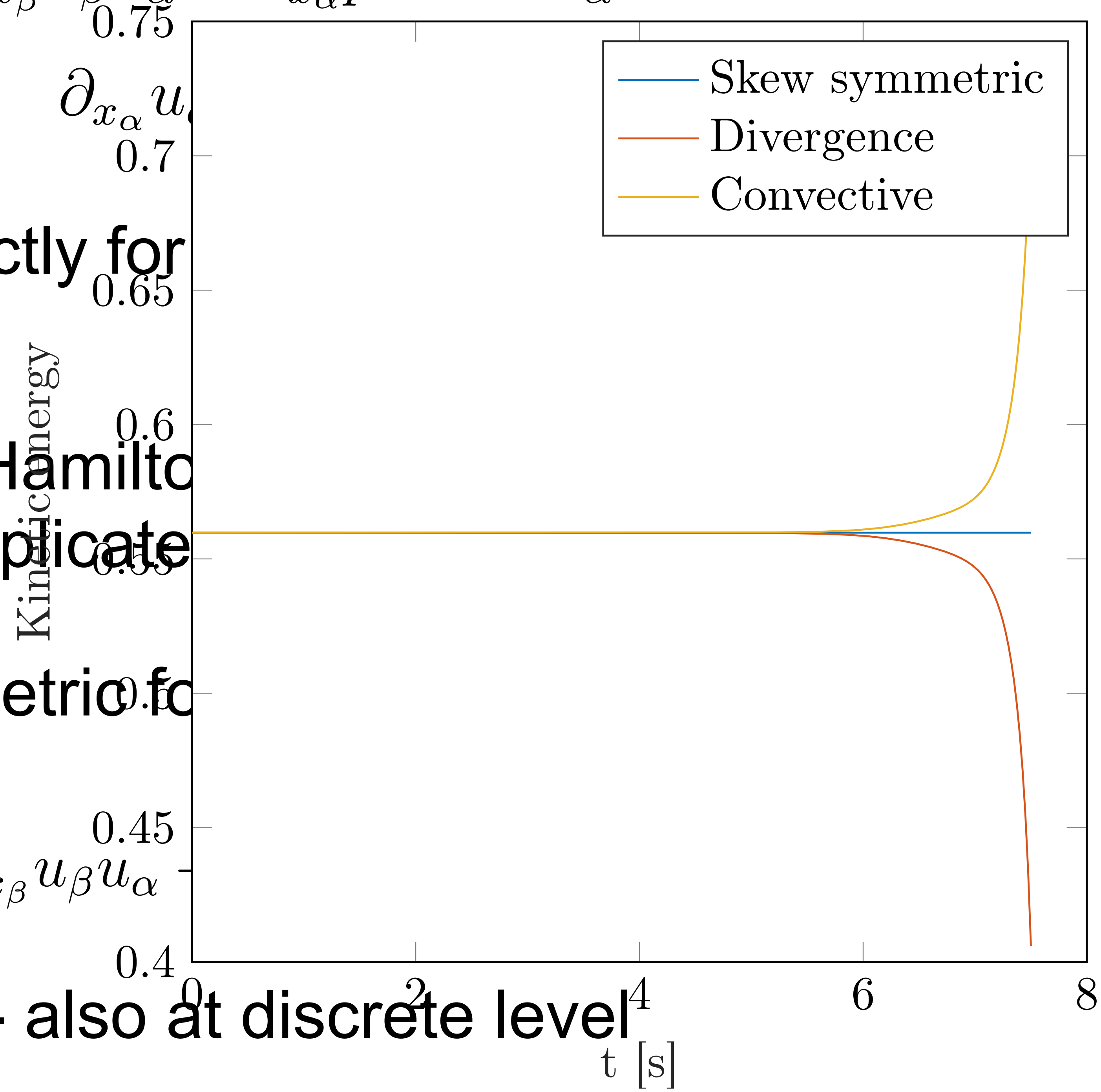


This conserves energy - also at discrete level

Euler/Navier-Stokes equations

To solve full model

- Asymmetric 7th order finite difference method
- Gauss collocation method (2nd and 4th order)

To integrate reduced model

- Gauss collocation method (2nd and 4th order)
- Nonlinearity addressed by EIM

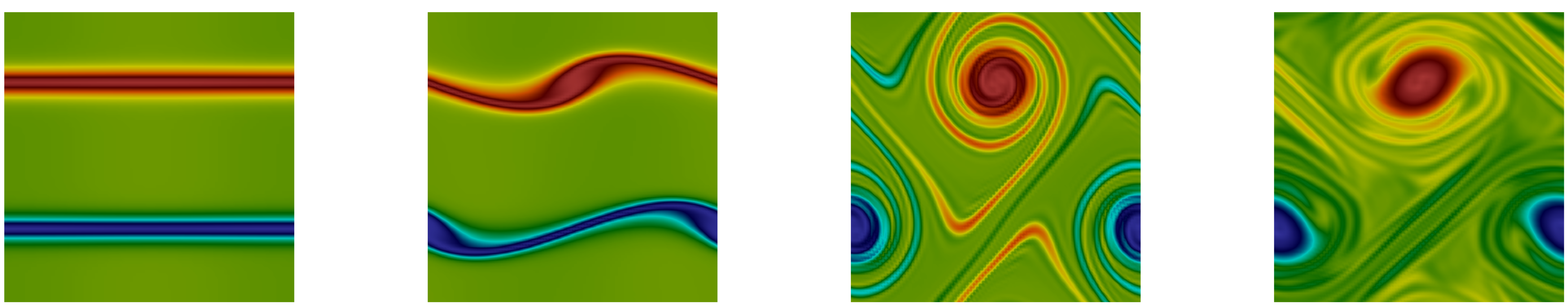
Euler/Navier-Stokes equations

Euler/Navier-Stokes equations

The double jet problem

$$\omega = \begin{cases} -\delta cos(x) - \frac{1}{\rho}\left(sech\left(y - \frac{\pi}{2}\right)\right)^2 & , \quad \text{if } y < \pi \\ -\delta cos(x) + \frac{1}{\rho}\left(sech\left(\frac{3}{2} - y\right)\right)^2 & , \quad \text{if } y > \pi \end{cases}$$

$\delta = 0.05$ and $\rho = \frac{\pi}{15}$.



Full model. N=100x100. T=0, 4, 10, 20

Euler/Navier-Stokes equations

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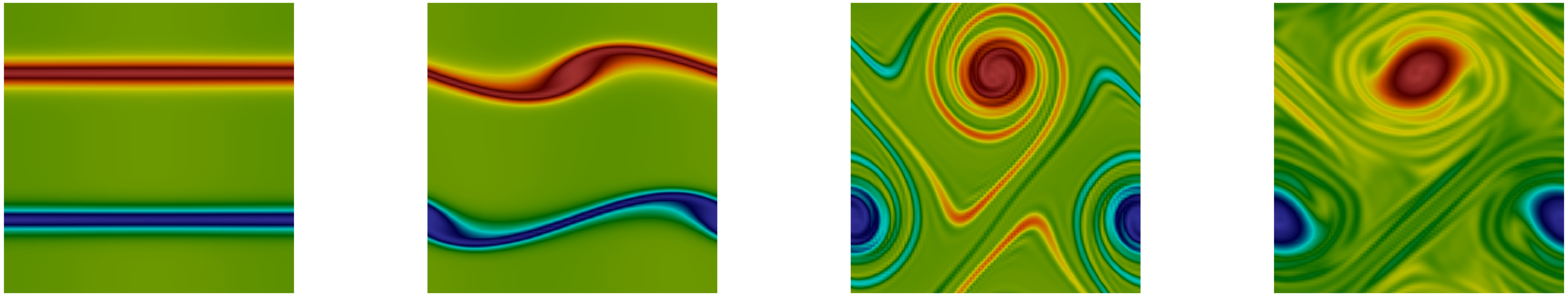
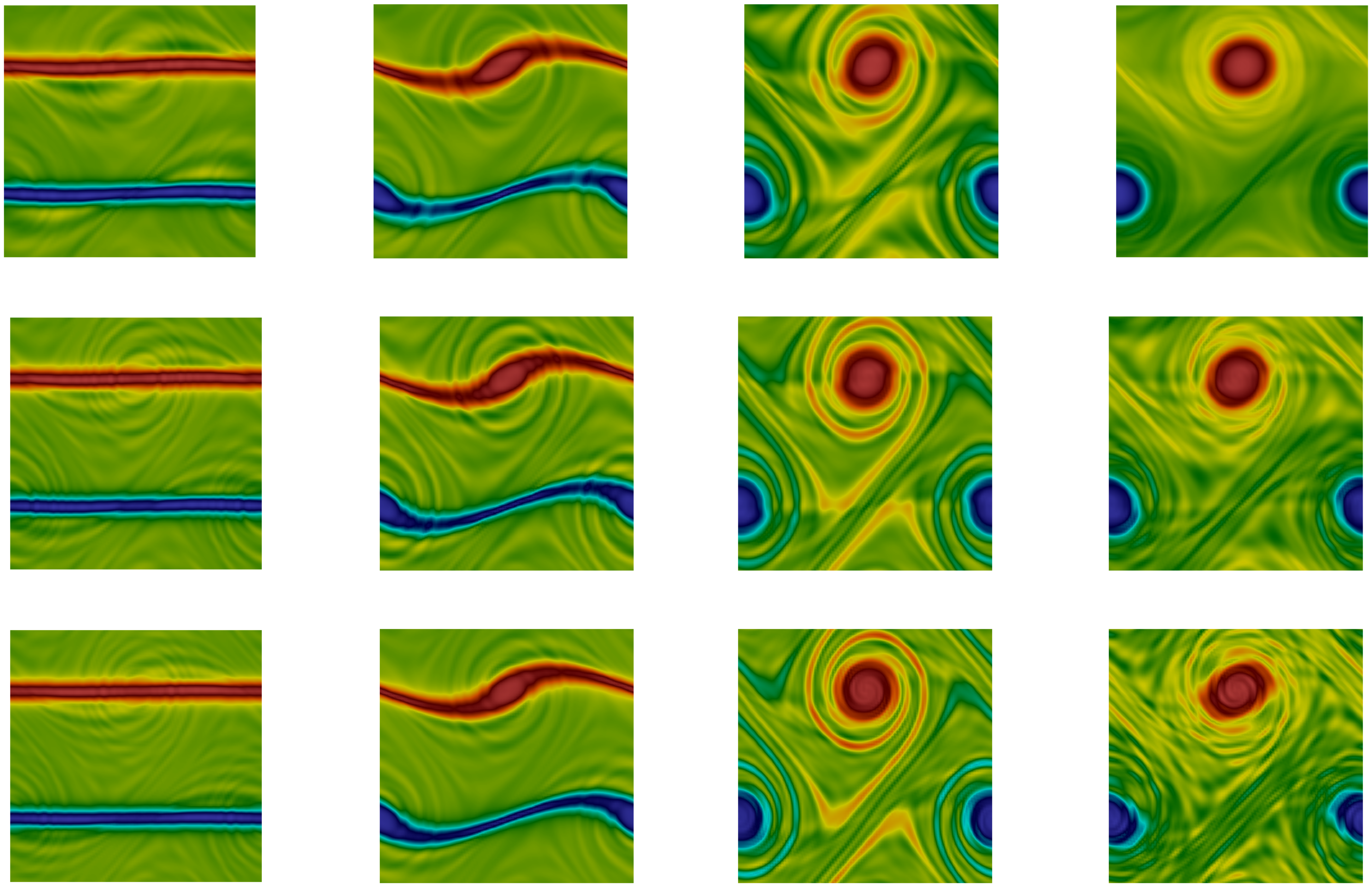


Euler/Navier-Stokes equations

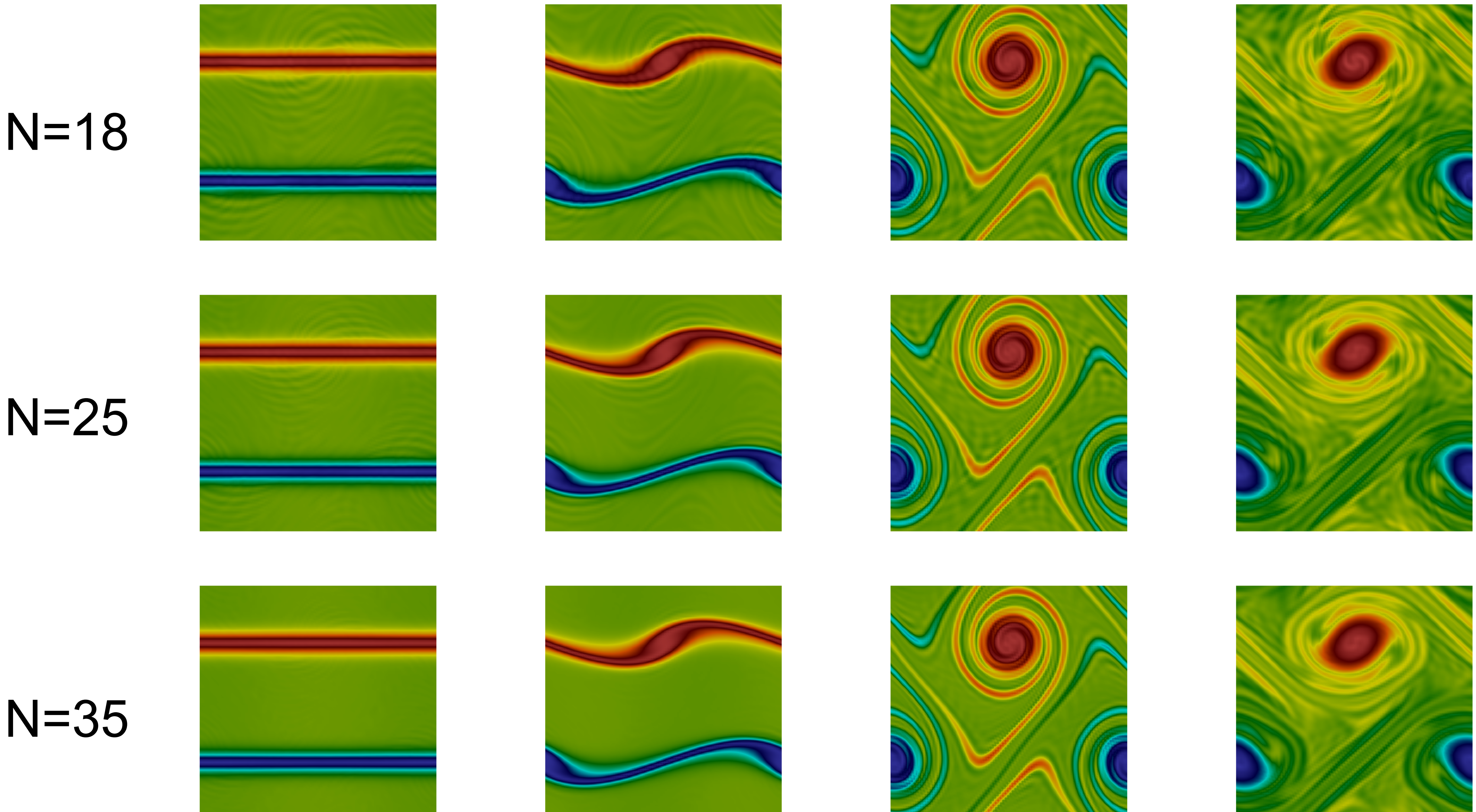


N=5

N=8

N=12

Euler/Navier-Stokes equations

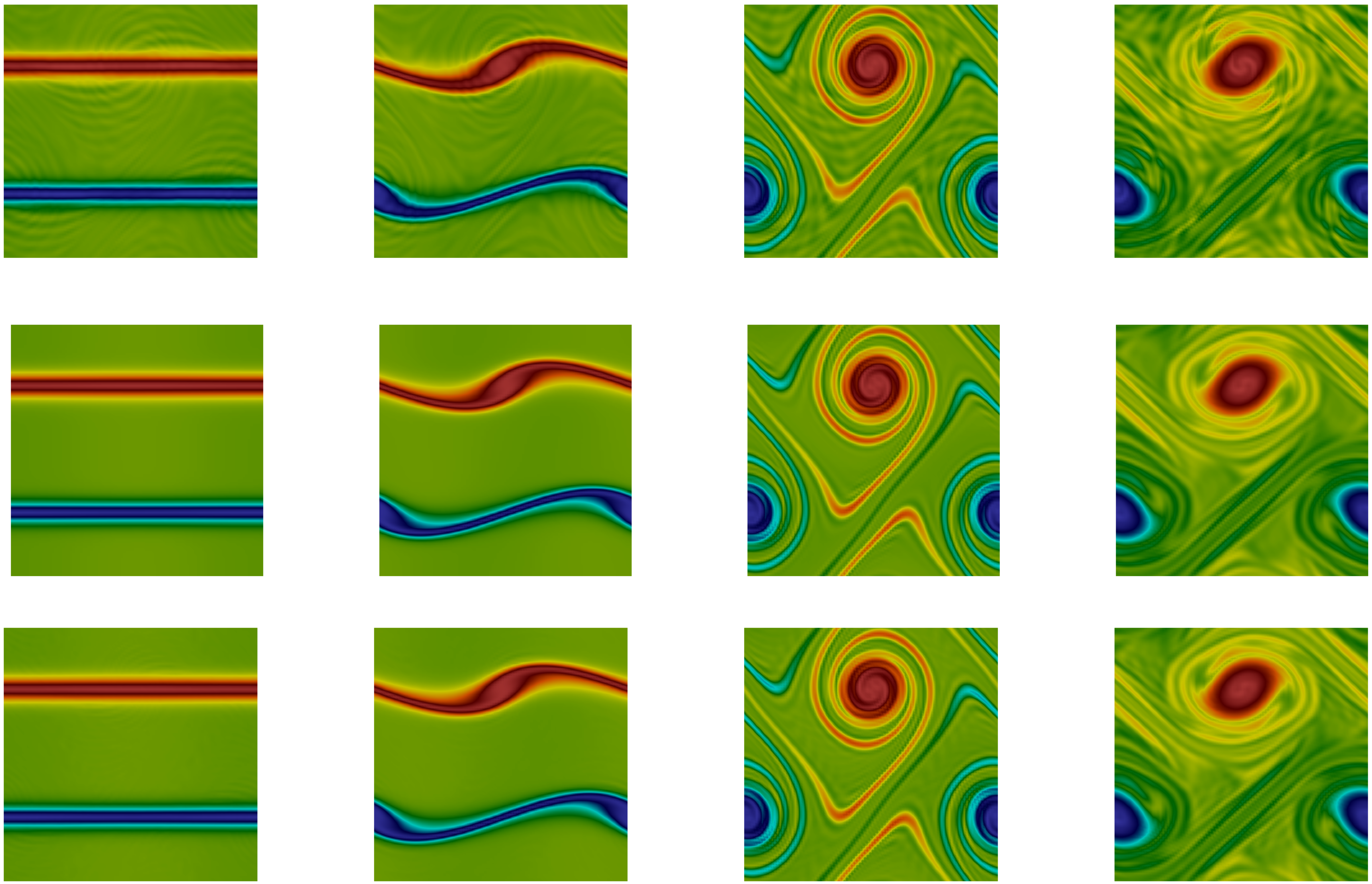


Euler/Navier-Stokes equations

N=18

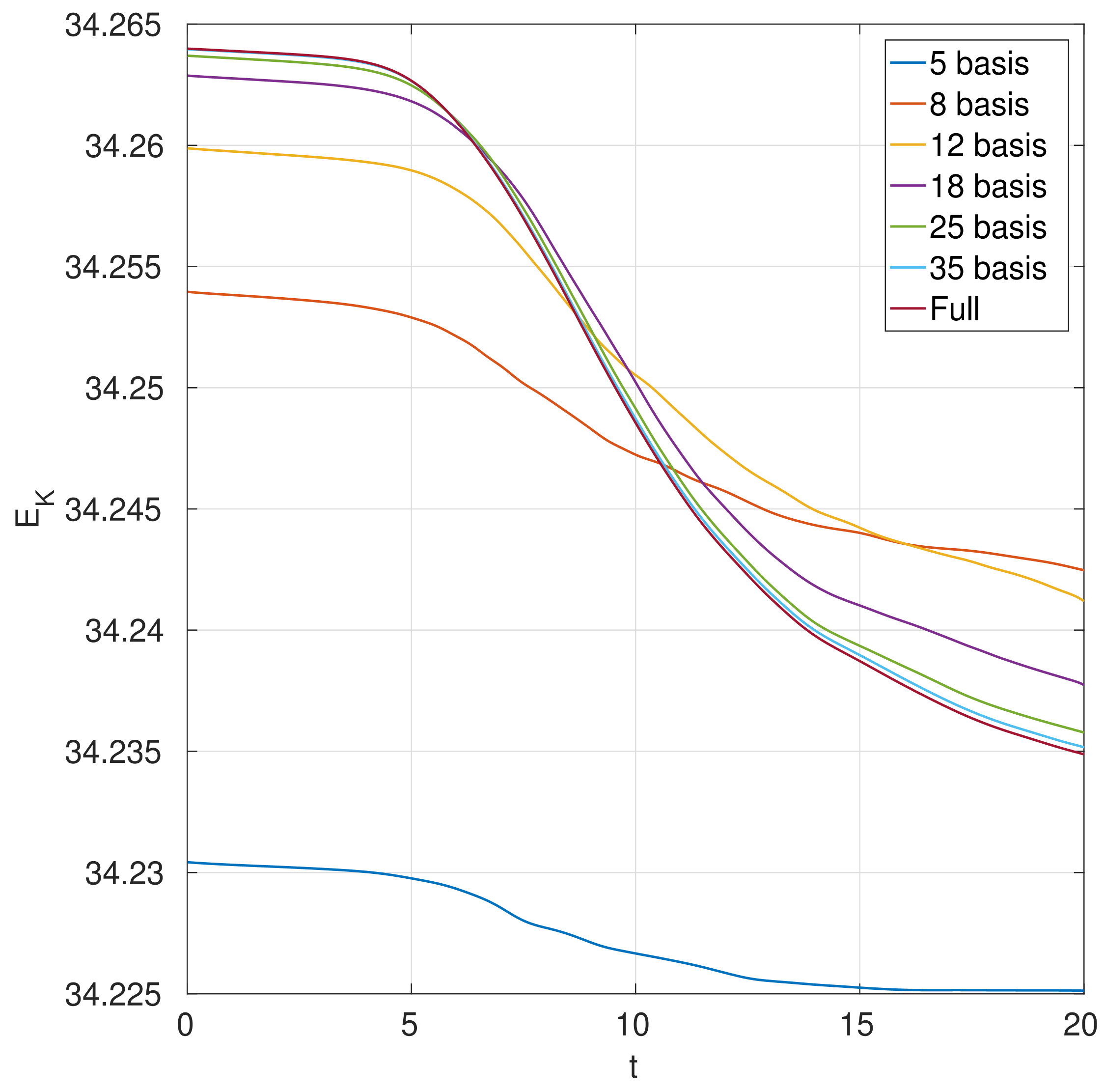
N=25

N=35



Euler/Navier-Stokes equations

Energy conservation



Euler/Navier-Stokes equations

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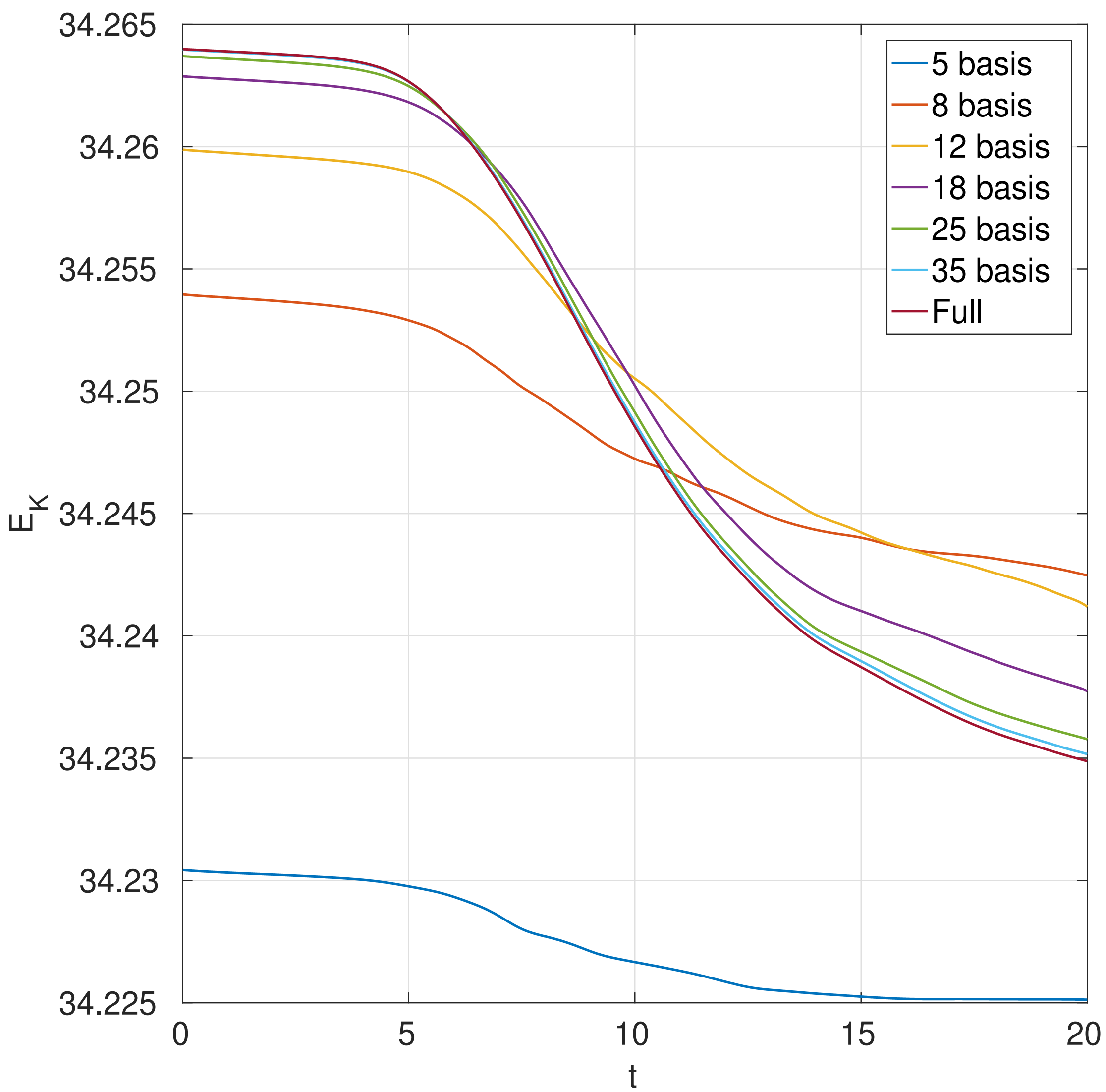

Cost

# basis	Reduced model (quadratic expansion)	% Full
5	1.18s	0.05%
8	1.38s	0.06%
12	1.99s	0.08%
18	3.91s	0.16%
25	8.44s	0.34%
35	16.69s	0.67%
Full	2480.13s	100%

Speedup ~ 1000

Euler/Navier-Stokes equations

Double vortex problem

$$\omega = -\alpha e^{-\frac{(x-\pi-d)^2+4(y-0.5\pi)^2}{4\pi\beta^2}} + \alpha e^{-\frac{(x-\pi+d)^2+4(y-0.5\pi)^2}{4\pi\beta^2}}$$

$\alpha = \frac{1}{4}\pi,\ \beta = 0.1 \text{ and } d = 0.65$

Full model. N=100x100. T=0, 20, 50, 100

Euler/Navier-Stokes equations

$$\omega = -\alpha e^{-\frac{(x-\pi-d)^2+4(y-0.5\pi)^2}{4\pi\beta^2}} + \alpha e^{-\frac{(x-\pi+d)^2+4(y-0.5\pi)^2}{4\pi\beta^2}}$$

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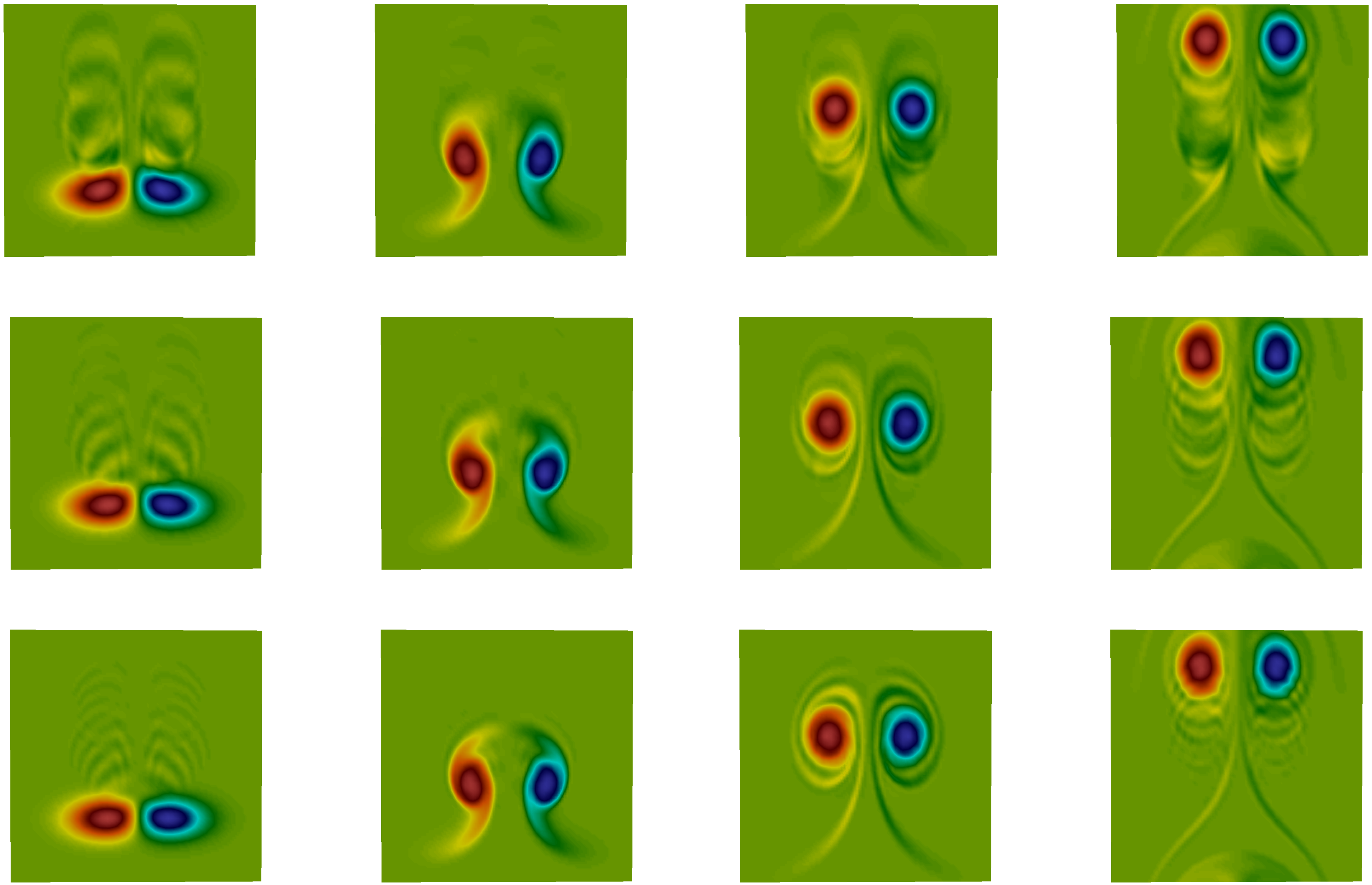
Euler/Navier-Stokes equations



N=5

N=8

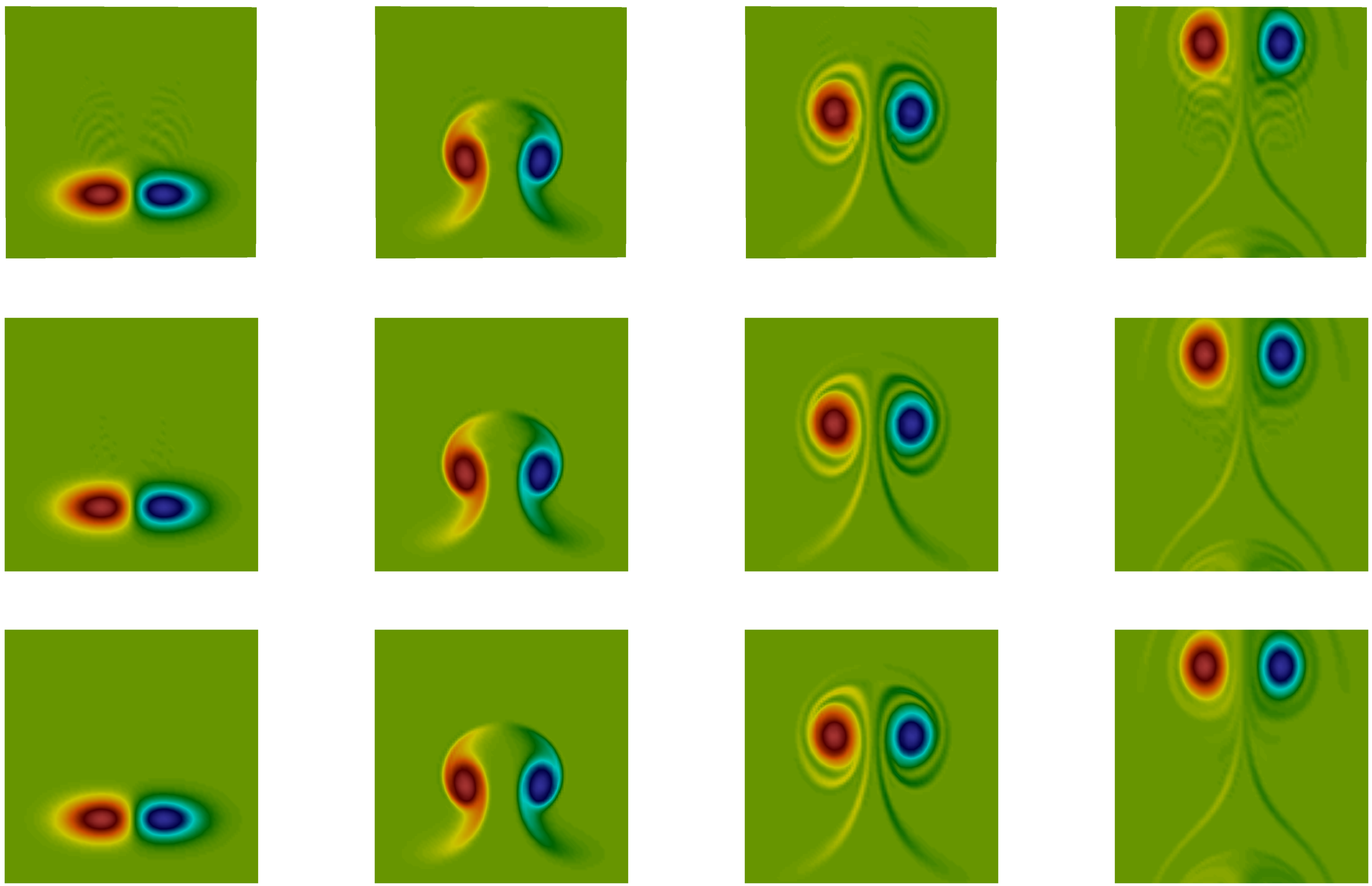
N=12

Euler/Navier-Stokes equations

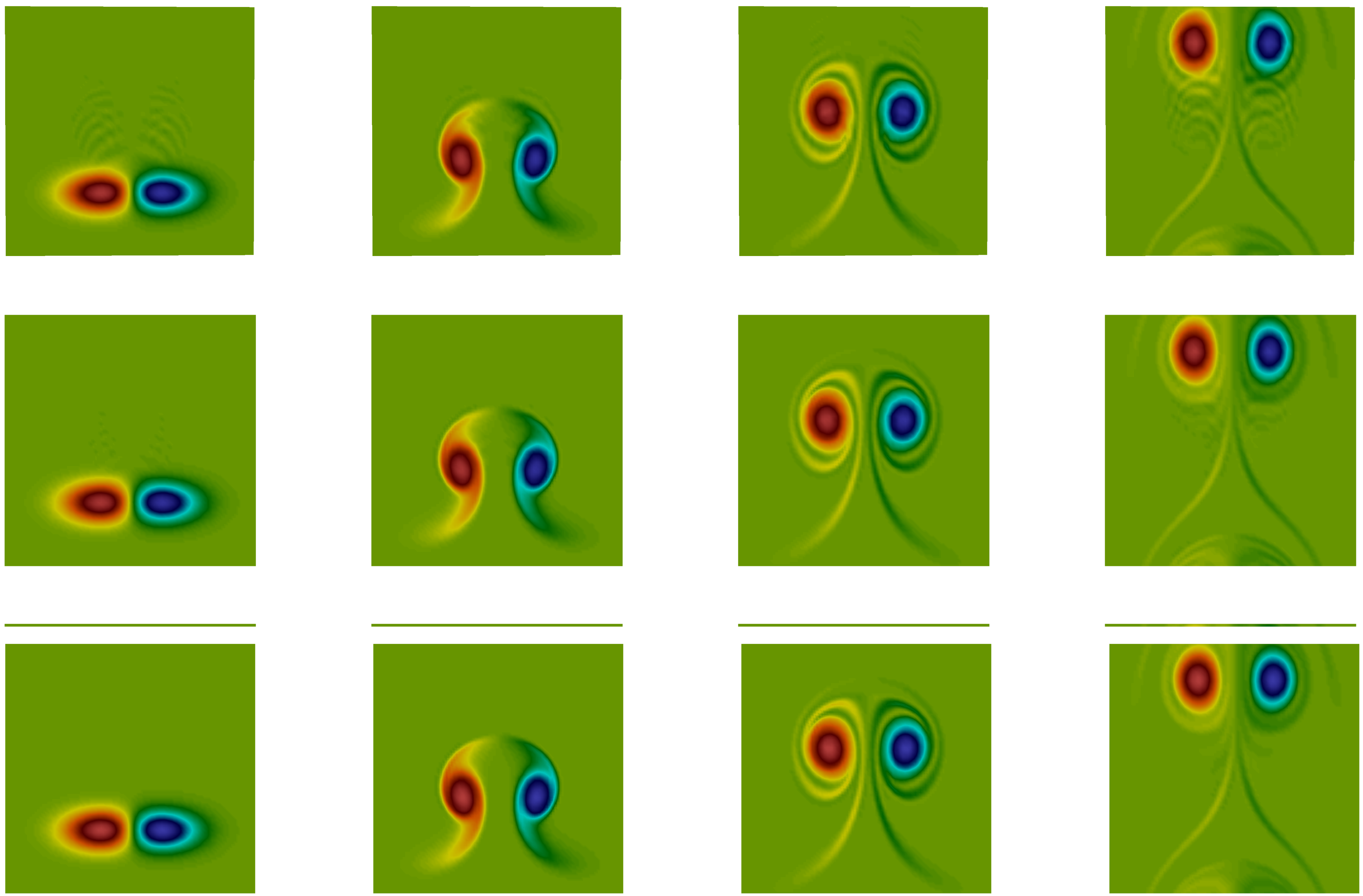
N=18

N=25

N=35



Euler/Navier-Stokes equations



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Euler/Navier-Stokes equations

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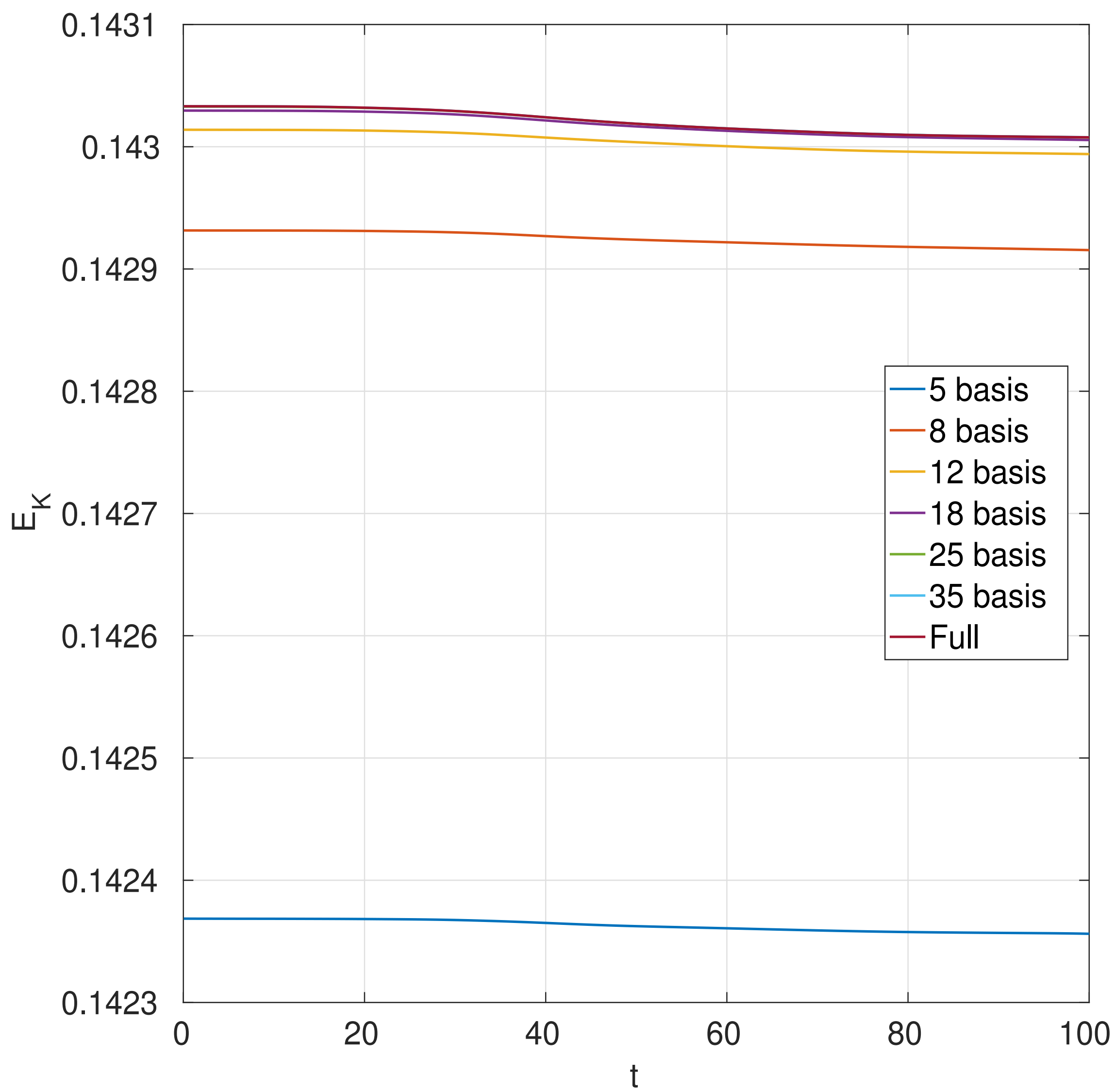
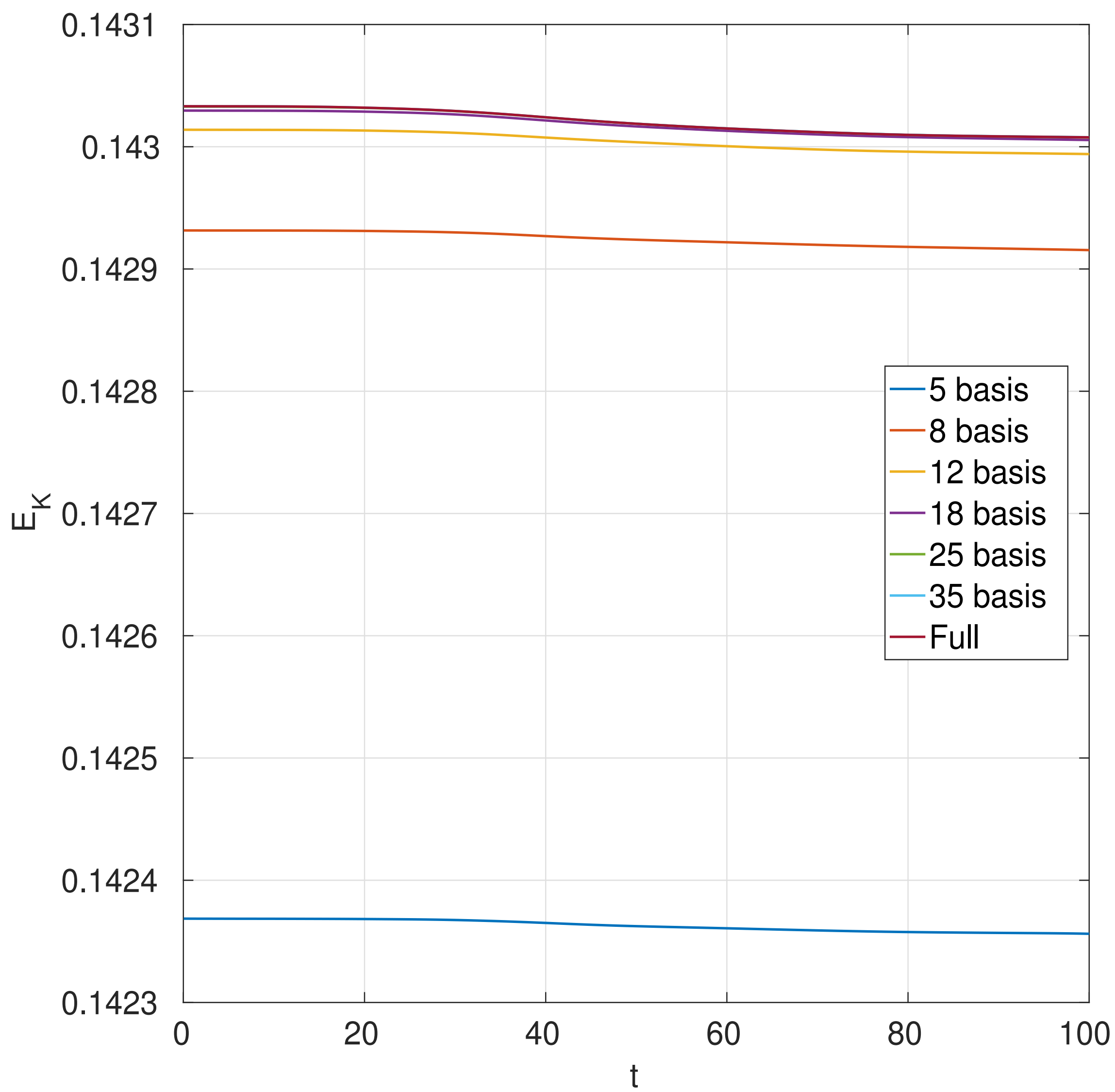


Euler/Navier-Stokes equations

Energy conservation



Cost

# basis	Reduced model (quadratic expansion)	% Full
5	0.93s	0.04%
8	1.15s	0.05%
12	1.67s	0.07%
18	3.30s	0.14%
25	6.22s	0.27%
35	14.06s	0.62%
Full	2280.94s	100%

Speedup ~ 1000

A brief summary

Status

- Reduced order models for time-dependent problems should not only be constructed for accuracy.
- The Hamiltonian approach offer some tools
- Greedy approach to construct basis
- Preservation of structure and invariants ensure stability
- Extension to linearly dissipative problems

Ongoing

- Extension to problems with several invariants
- More general dissipative models
- Generalizations to conservation laws