Machine Learning of Transport Phenomena Simulated by Reduced-Order Models Based on Proper Orthogonal Decomposition

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Outline

- Motivation and Current Limitations
- Proper Orthogonal Decomposition (POD)-based Reduced-order Models
- Machine Learning
- Results
  - Nozzle Flow
  - Compressible Gas-Only Flow in Reactor
  - Gas-Solids Dynamics in a Fluidized Bed
- Conclusions and Future Work

Motivation

- Computational Fluid Dynamics prediction of transport phenomena is computationally expensive
- Reduced-order modeling is an appealing alternative to full-order modeling
- Proper orthogonal decomposition can reduce computational time by 10,000[1] times or more, but it is not trivial to implement
- Machine learning is promising, but reacting two-phase flows are much more challenging than face recognition

[1] Elizabeth Krath, Forrest Carpenter, and Paul Cizmas. "Prediction of unsteady flows in turbomachinery cascades using proper orthogonal decomposition" in: Physics of Fluids 36.3 (Mar. 2024)

Proper Orthogonal Decomposition (POD) Method

- POD is also known as Singular Value Decomposition, Karhunen-Loeve Decomposition, Principal Components Analysis, and Singular Systems Analysis
- Provides optimal basis for modal decomposition of a data set
- Extracts key **spatial** features from physical systems with spatial and temporal characteristics
- Reduces a large set of governing PDEs to a much smaller set of ODEs

POD Method

- Extracts:
  - time-independent orthonormal basis functions $\varphi_k(x)$
  - time-dependent orthonormal amplitude coefficients $\alpha_k(t_i)$ such that the reconstruction
  - $$u(\mathbf{x}, t_i) = \sum_{k=1}^{M} \alpha_k(t_i)\varphi_k(\mathbf{x}), \qquad i = 1,\ldots, M$$
  - is optimal in the sense that the average least square truncation error
  - $$\epsilon_m = \langle \| u(\mathbf{x}, t_i) - \sum_{k=1}^{m} \alpha_k(t_i)\varphi_k(\mathbf{x}) \|^2 \rangle \qquad (1)$$
  - is a minimum for any given number $m \le M$ of basis functions over all possible sets of orthogonal functions

POD Method

- Optimal property (1) reduces to
- $$\int_D \langle u(x)\ u^*(y)\rangle \varphi(y) dy = \lambda \varphi(x) \qquad (2)$$

φ_k are eigenfunctions of integral equation (2), whose kernel is the averaged autocorrelation function

$$\langle u(\mathbf{x})\ u^*(\mathbf{y})\rangle \equiv R(\mathbf{x}, \mathbf{y}) \qquad (3)$$

- For a finite-dimensional case, (3) replaced by tensor product matrix
- $$\overline{\overline{R}} = \frac{\sum_{i=1}^{M} u(\mathbf{x}, t_i)\ u^T(\mathbf{y}, t_i)}{M}$$

POD Steps

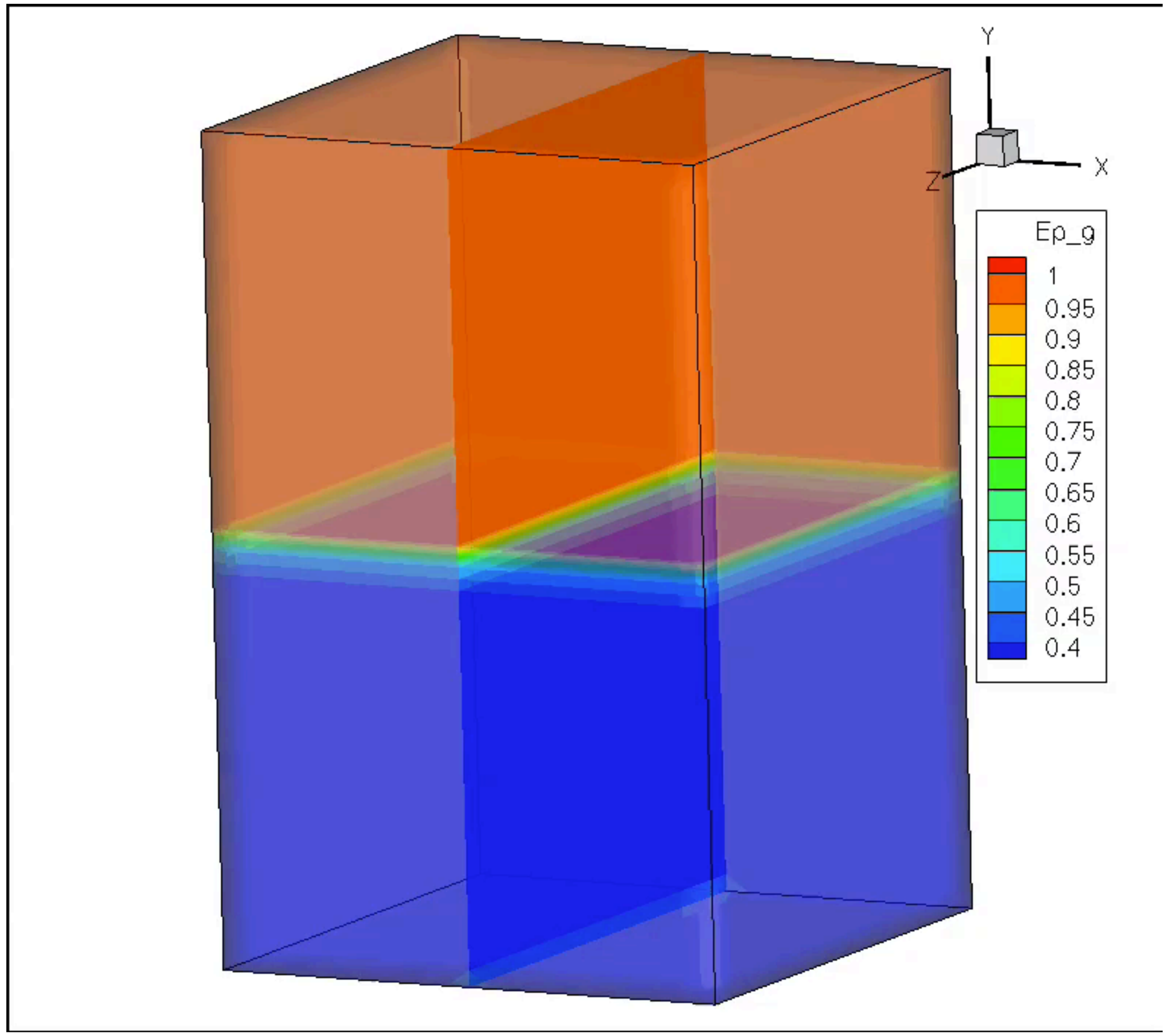
- Generate database using full-order model
- Assembly autocorrelation matrix and extract eigenmodes
- Substitute approximation in governing equations and perform Galerkin projection
- Solve ODE system to obtain time coefficients and reconstruct solution

OTHER POD-Like Reduced-Order Models

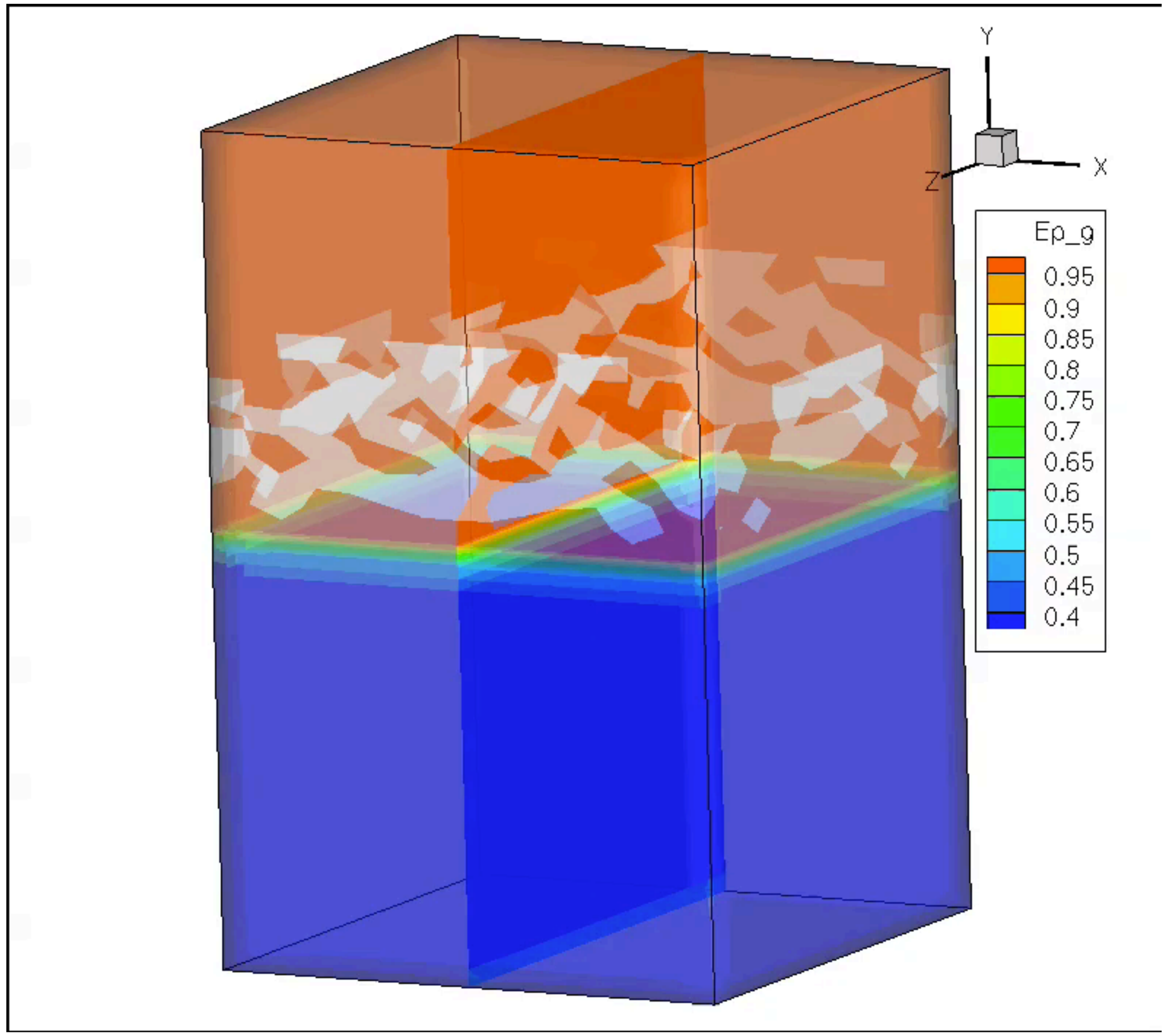
- Bi-orthogonal Decomposition (Audry, 1991)
- Balanced Proper Orthogonal Decomposition (Rowley, 2005)
- Dynamic Mode Decomposition (Schmid, 2010)
- Dynamic Proper Orthogonal Decomposition (Freno & Cizmas, 2015)
- Constraint Proper Orthogonal Decomposition (Cizmas *et al.*, 2017)
- Zeta Proper Orthogonal Decomposition (Cizmas *et al.*, JCP 2021, PoF 2024)

Void Fraction, ϵ_G

Full-order model



Reduced-order model



Computational Time - Zeta-POD

Case	Rotor 67	10 SC	11 SC
Grid nodes, N	299,844	33,068	78,260
Snapshots per Period	50	100	100
Total Snapshots	250	500	500
FOM Snapshots [s]	388,891	473,059	2,260,688
POD Basis Functions [s]	479	173	397
POD Basis/FOM Snapshots	0.12%	0.04%	0.02%

CPU runtime: FOM vs ROM

Case	N	M	FOM [s]	ROM [s]	Ratio
Rotor 67	299,844	250	4,860,247	51.30	94,749
10 SC	33,068	500	530,558	12.46	42,580
11 SC	78,260	500	2,260,688	24.35	92,841

Elizabeth Krath, Forrest Carpenter, and Paul Cizmas. “Prediction of unsteady flows in turbomachinery cascades using proper orthogonal decomposition” in: Physics of Fluids 36.3 (Mar. 2024)

Machine Learning (ML)

- Machine Learning = *automated* data analysis during which computer programs (or models) are learned from data
- Model (or computer program) describes relationship between variables (or data) and properties of interest, e.g., void fraction, solids particle velocity
- Model is learned using training data by using a learning algorithm that automatically adjust parameters of model to agree with data
- Cornerstones of machine learning: (1) data, (2) model, and (3) learning algorithm

Approach

- POD basis functions $\varphi_i(\mathbf{x})$ are known; only unknowns are time coefficients $\alpha_i(t)$
- Apply machine learning to find time coefficients $\alpha_i(t)$ of POD approximation
- Use snapshots as training data for $\alpha_i(t)$

Machine Learning Methodology

- Use of POD basis functions ensures time coefficient data is optimal
- Learn instantaneous time rates of change of POD time coefficients
- ML can identify latent ODE that governs POD time coefficients
- Usually achieved using recurrent neural networks (RNN) or residual neural networks (ResNet)
- Instead use neural ODE (NODE) machine learning algorithm

Neural Ordinary Differential Equations

- RNN and ResNet learn Euler time integration
- NODE network is integrated using time integration scheme of choice
- Backpropagation is possible for many integration schemes
- Allows model to learn under high-order and/or adaptive time integration
- NODE networks can outperform similarly sized RNN and ResNet by several orders of magnitude

Tasks

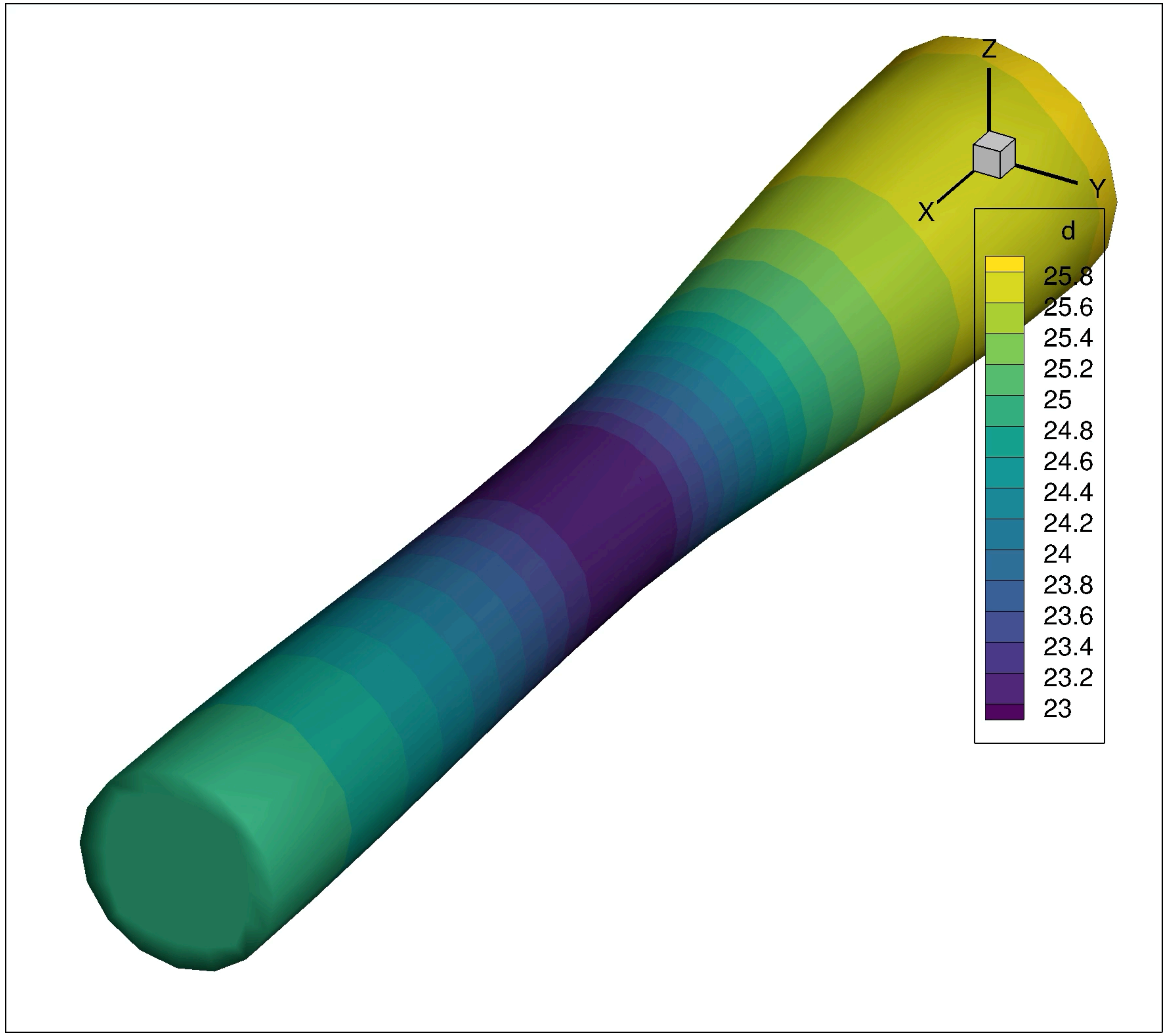
- Generate training data
- Assemble autocorrelation matrix $\overline{\overline{R}}$, calculate POD basis functions $\varphi_i(\mathbf{x})$
- Use machine learning to determine time coefficients $\alpha_i(t)$
- Reconstruct solution $u(\mathbf{x}, t)$ for on- and off-reference conditions
- Compare machine learning results vs. POD results

Machine Learning Results

- Flow through nozzle
- Compressible gas-only flow in a reactor
- Gas-solids dynamics in a fluidized bed

Flow Through Nozzle

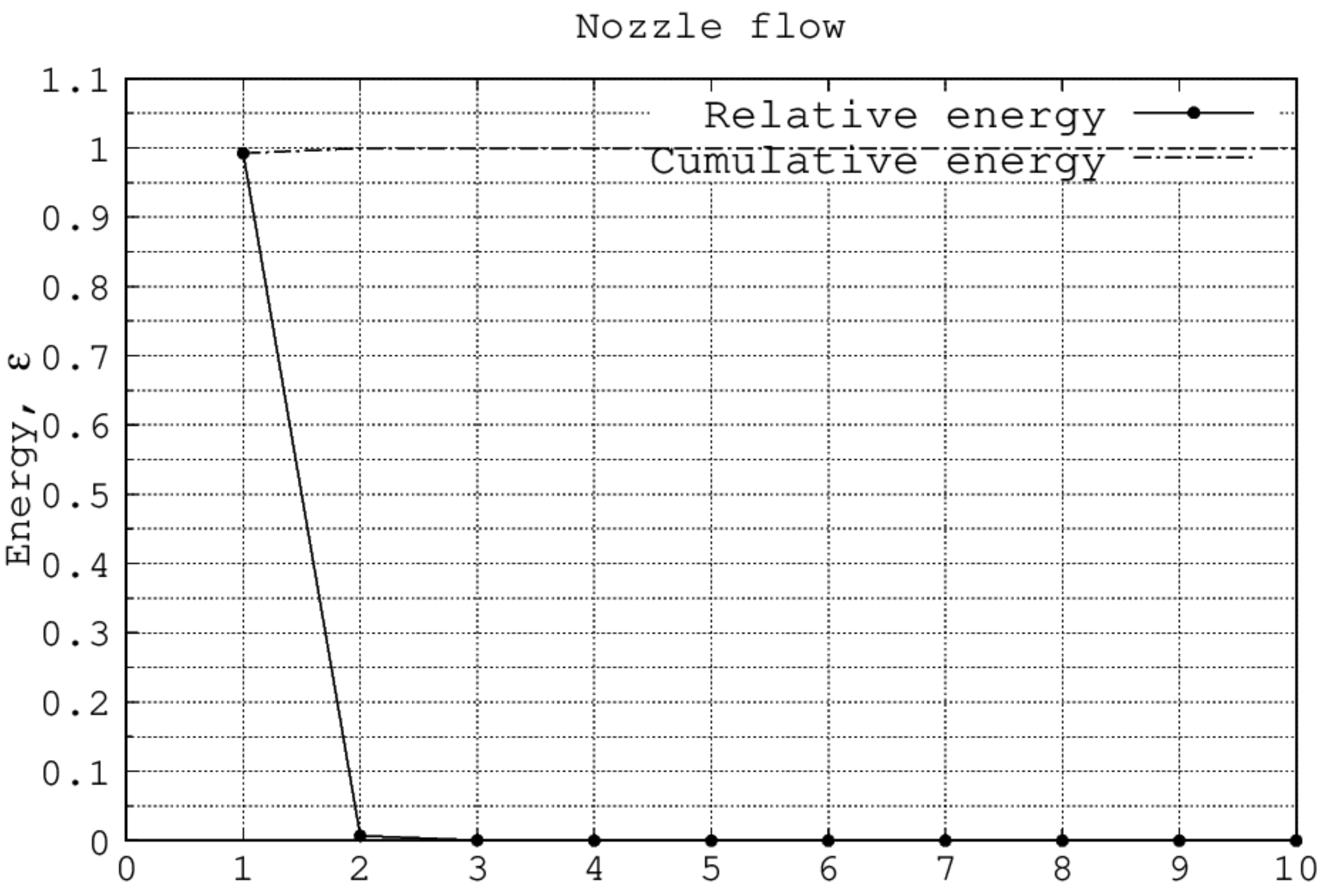
Nozzle with Varying Back Pressure



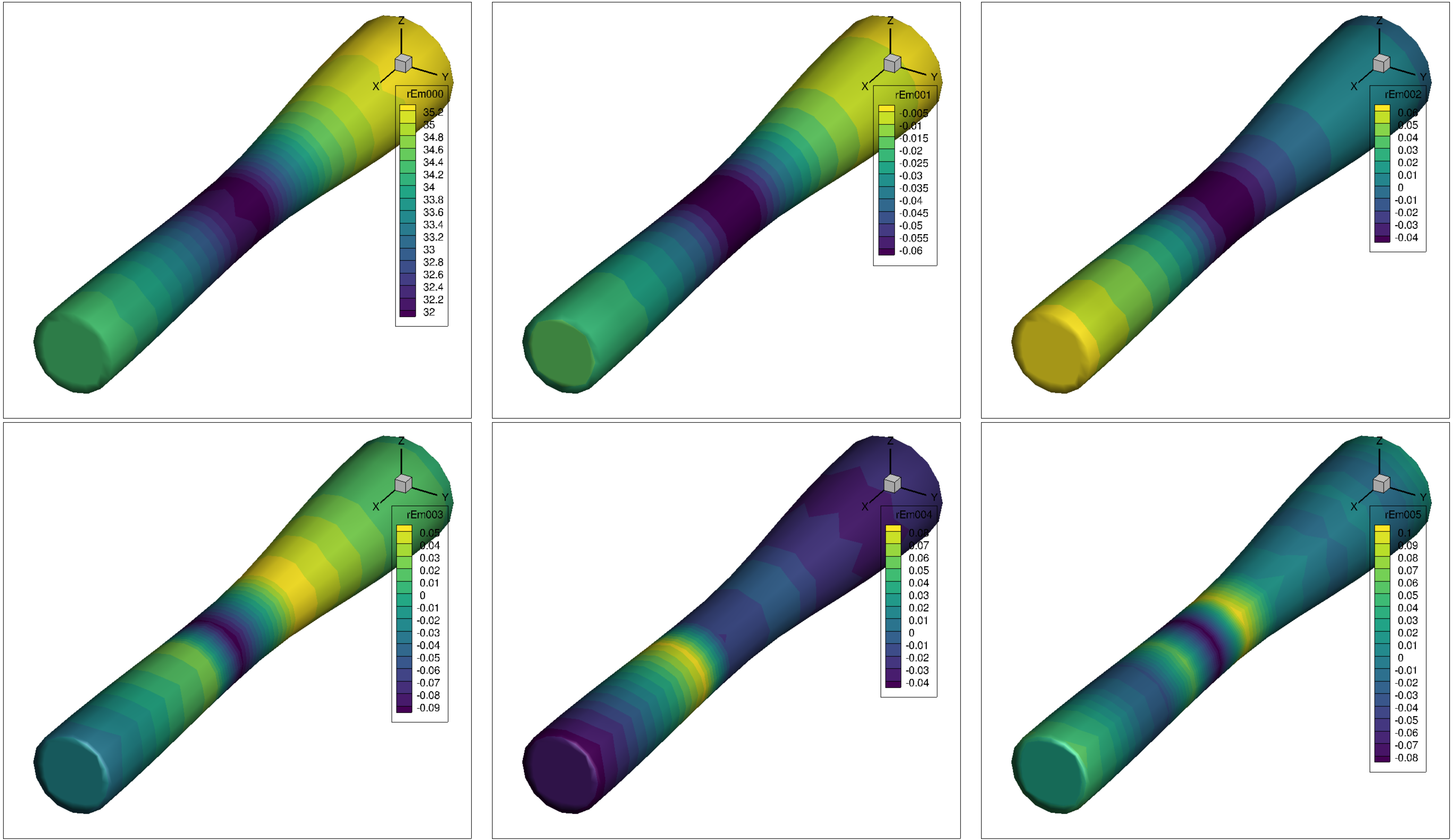
Case	Ampl.	
1	0	On
2	0.1	On
3	0.2	On
4	0.3	On
5	0.4	On
6	0.5	On
7	0.25	Off
8	0.45	Off

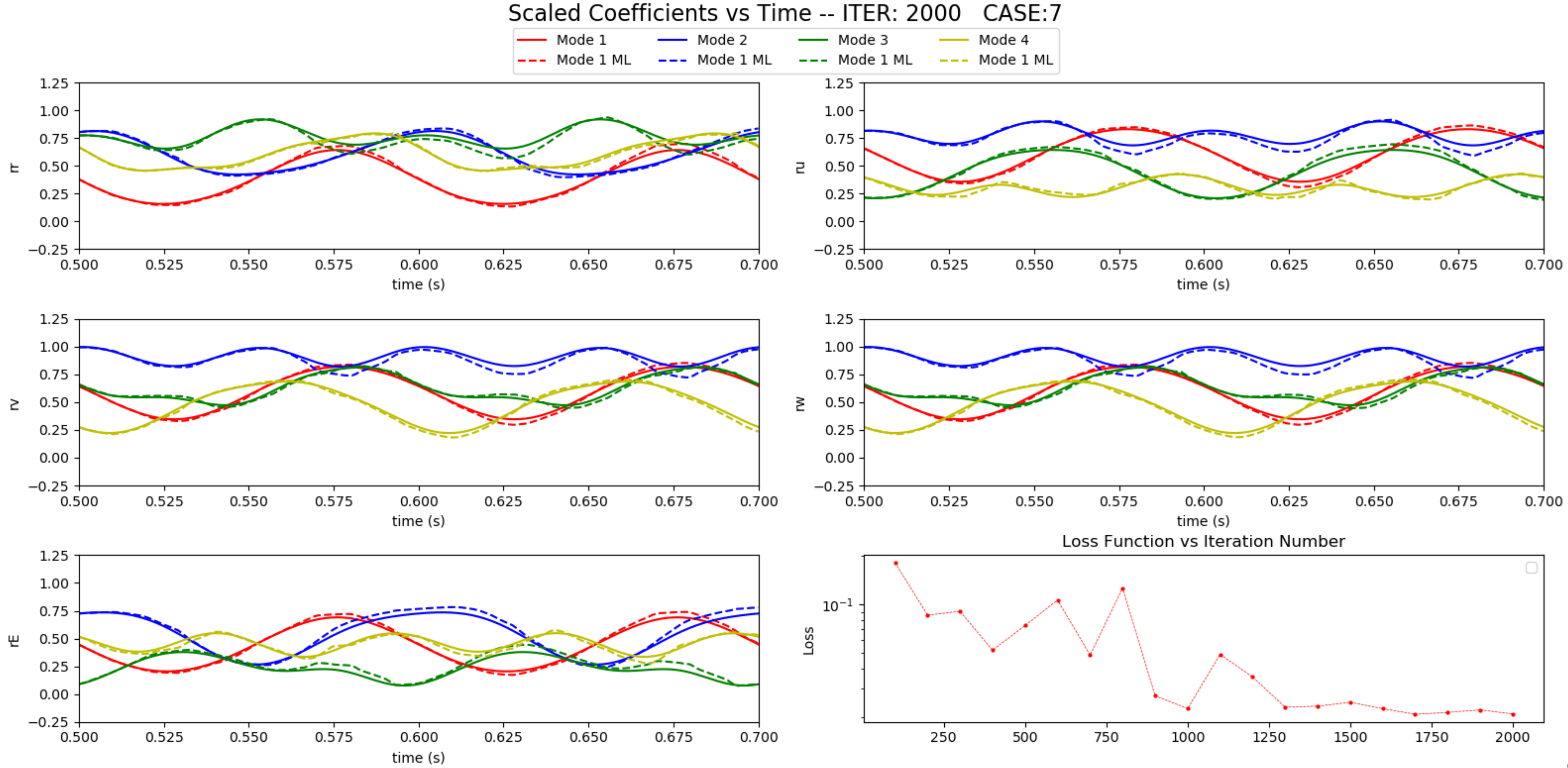
Energy Spectrum of Energy

1	0.99226345051693110	0.99226345051693110
2	7.1410038886774050E-003	0.99940445440560854
3	5.7316278605065653E-004	0.99997761719165923
4	1.8245441422569632E-005	0.99999586263308182
5	3.2021417412744801E-006	0.99999906477482314
6	7.2616041087253879E-007	0.99999979093523406
7	1.6994246506351193E-007	0.99999996087769916
8	3.0709907075445557E-008	0.99999999158760622
9	6.9899374814050319E-009	0.99999999857754374
10	8.2645864761026812E-010	0.99999999940400242
11	4.4514043716615689E-010	0.99999999984914290
12	7.8535765252173596E-011	0.99999999992767863
13	5.5933822544949732E-011	0.99999999998361244
14	9.6411515599660522E-012	0.99999999999325362

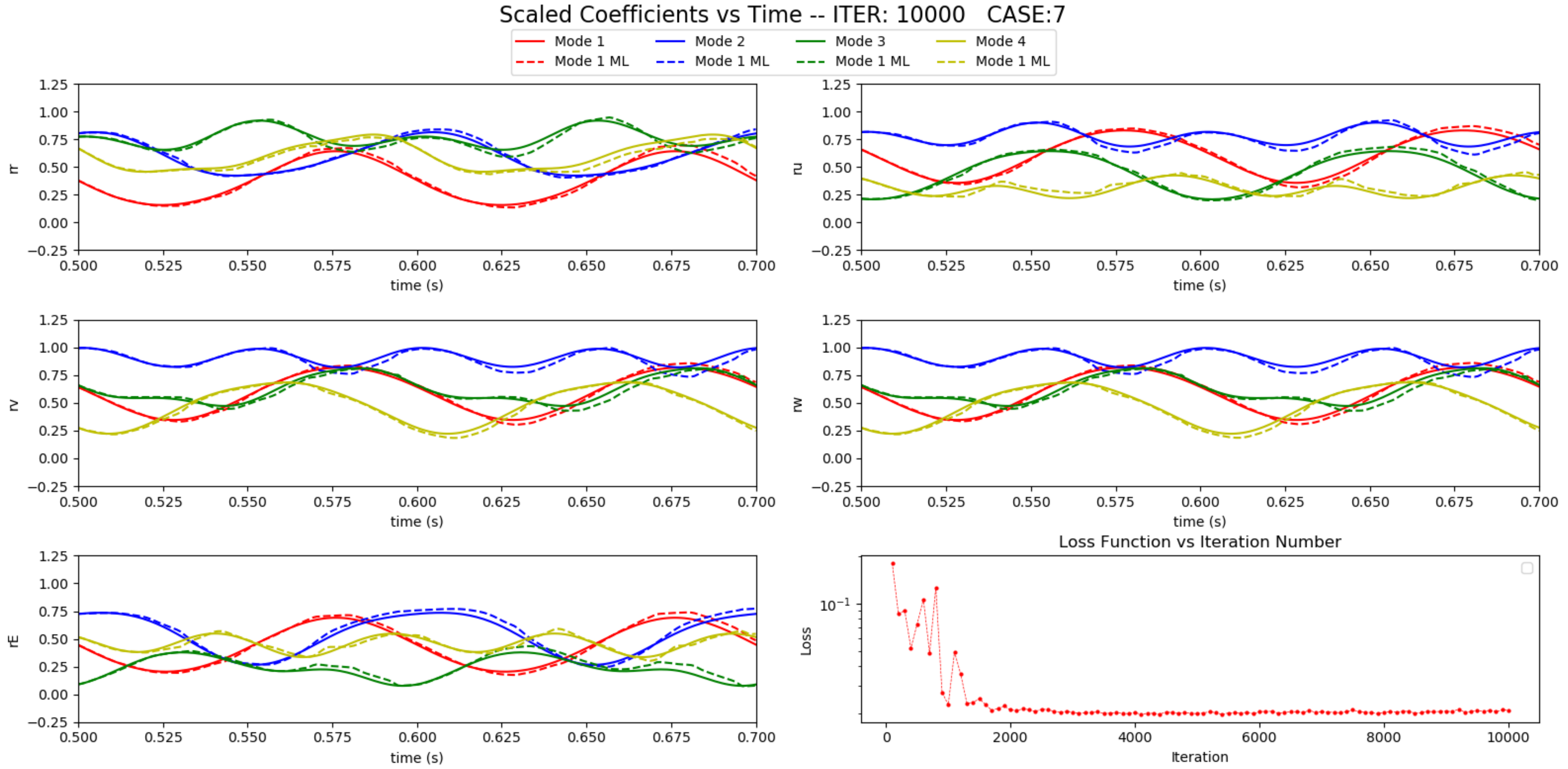


Energy Modes



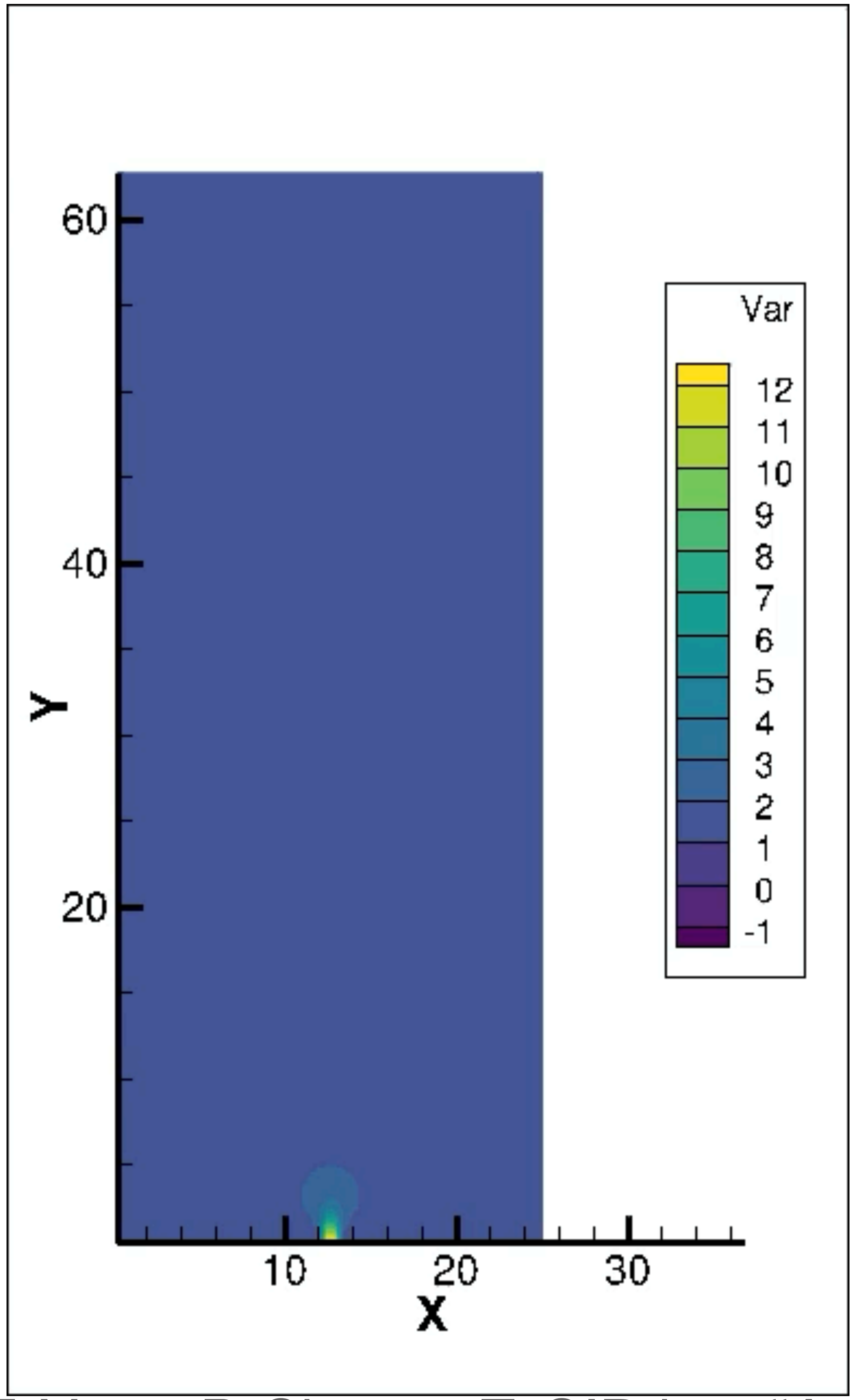


Off-Reference Case 7

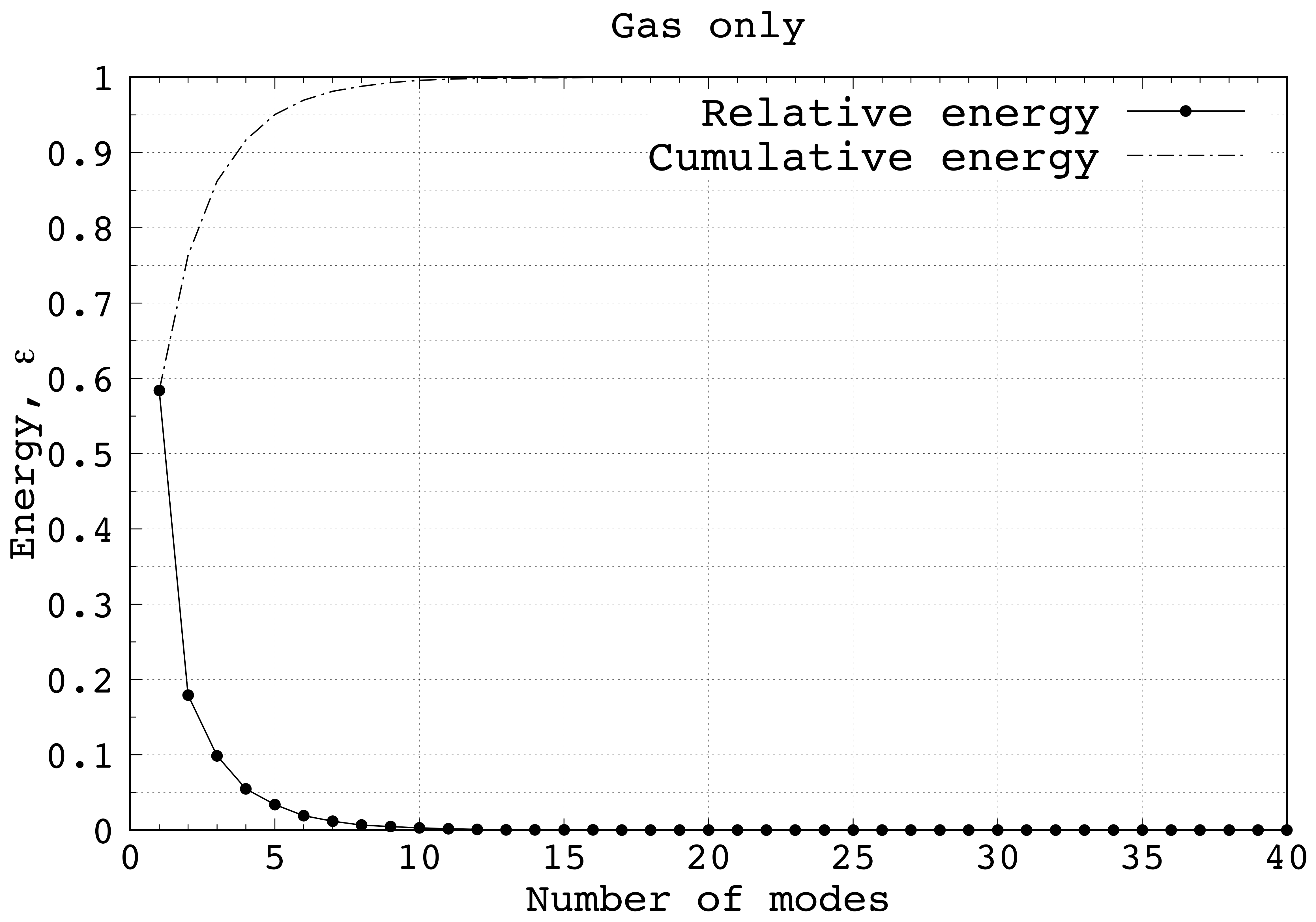


Compressible Gas-Only Flow

Gas Only - V Velocity



Case	V_jet	
1	11.4	On
2	12.0	On
3	12.6	On
4	13.2	On
5	13.9	On
6	13.0	Off

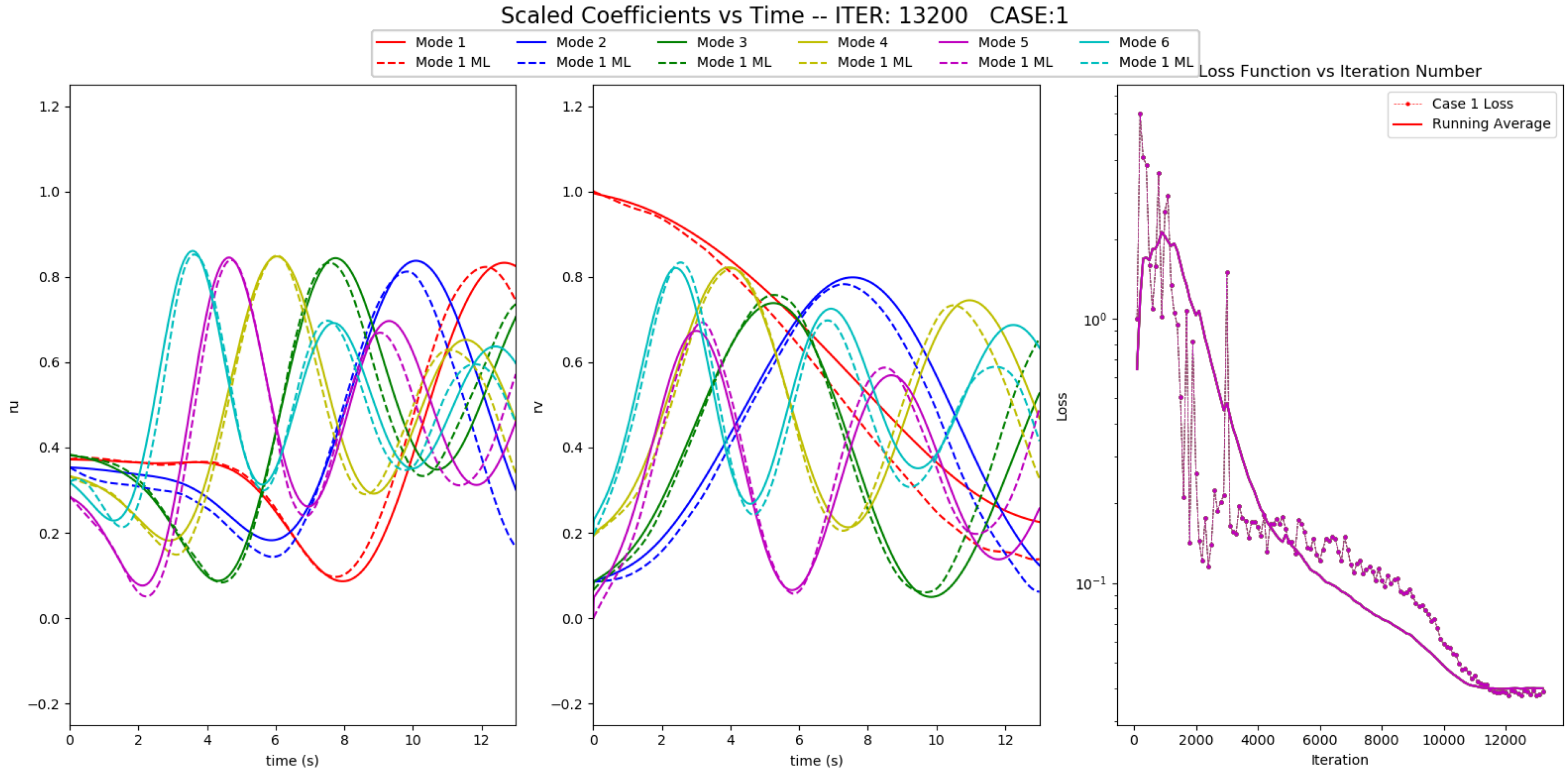


T. Yuan, P. Cizmas, T. O'Brien, "A reduced-order model for a bubbling fluidized bed bases on proper orthogonal decomposition, Computers & Chemical Engineering, 30, 2005.

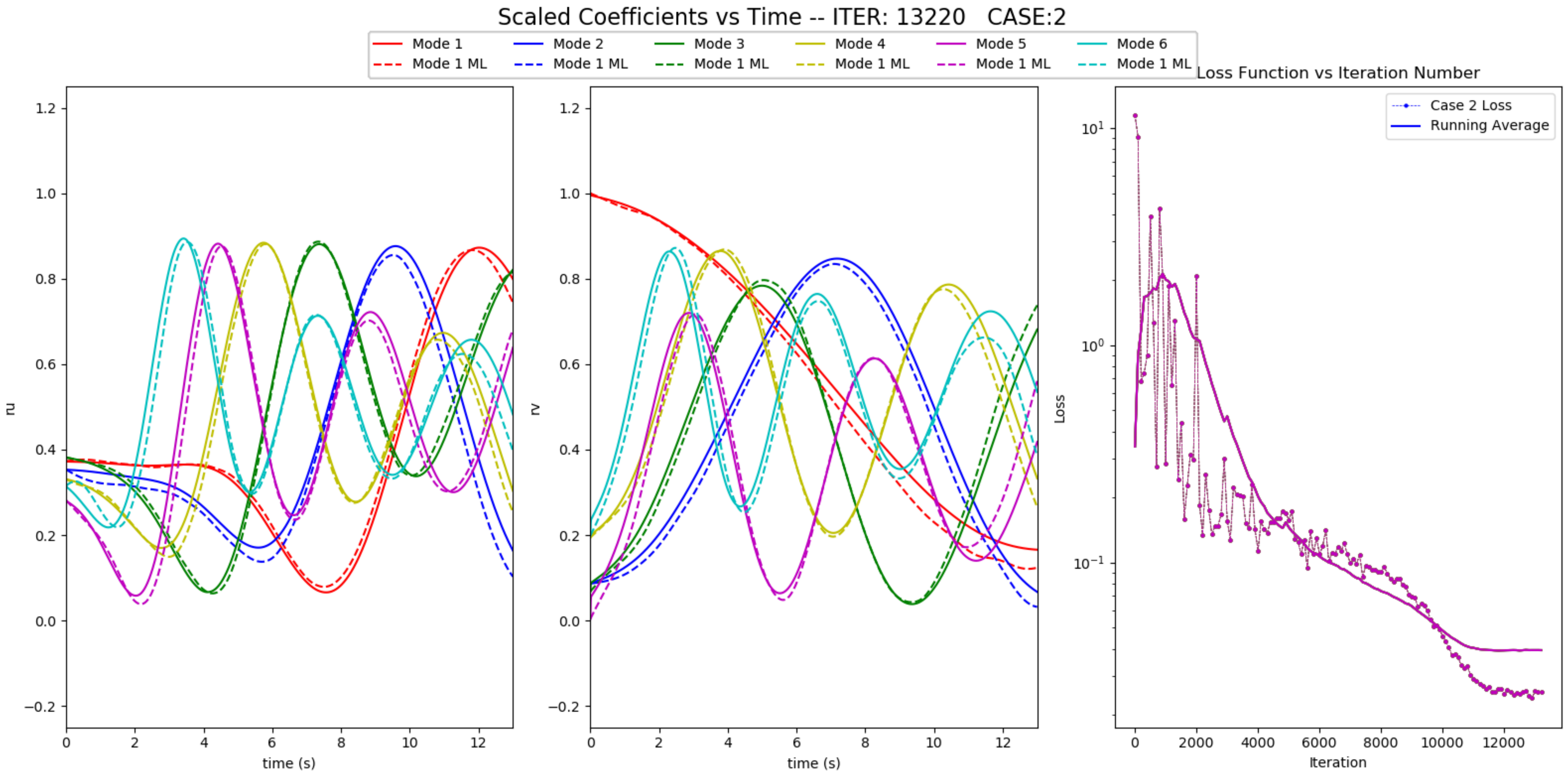
Gas Only - POD Modes of V Velocity

0 1 2 3 4

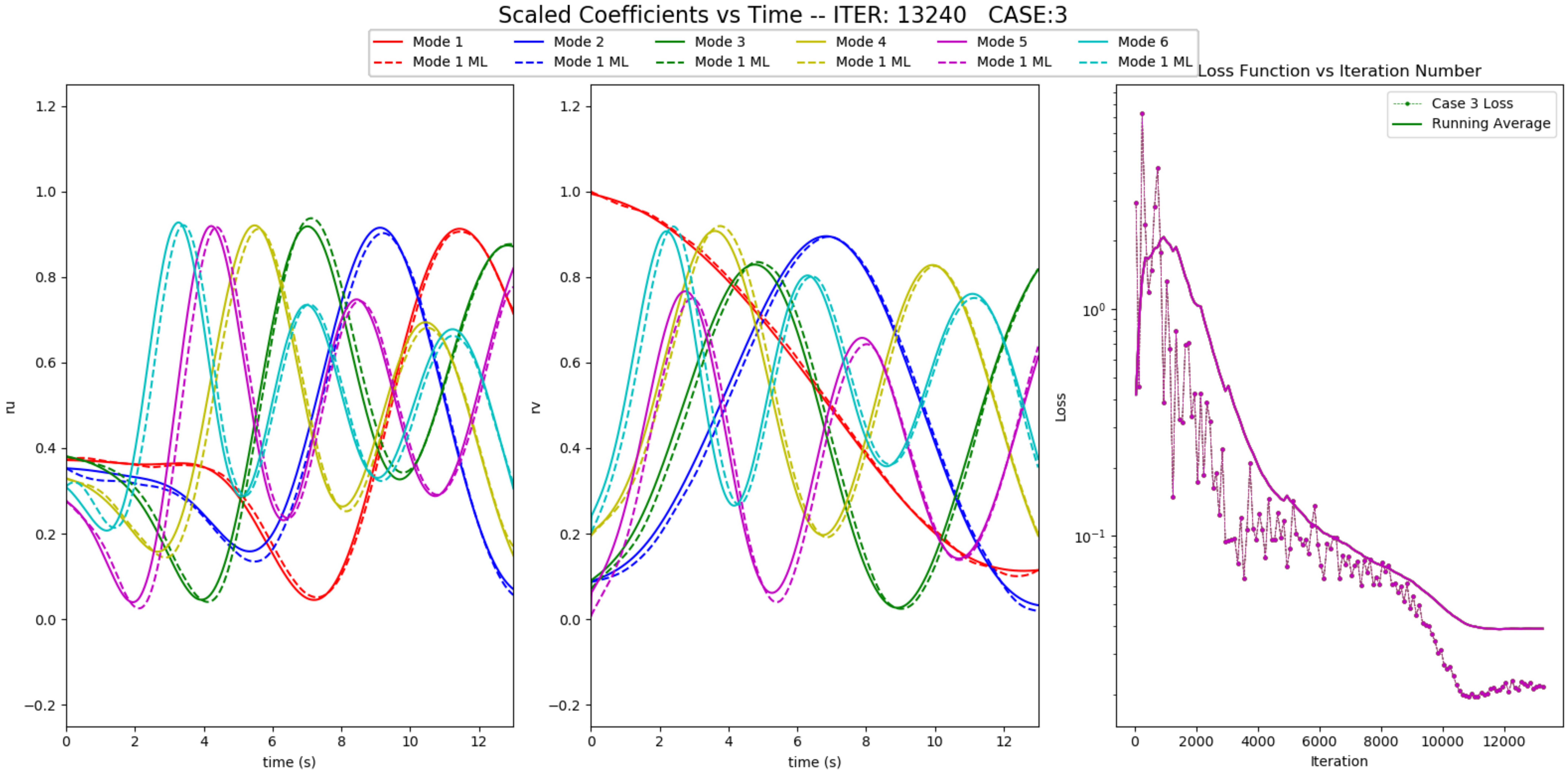
ML vs POD, Case 1, 13 seconds



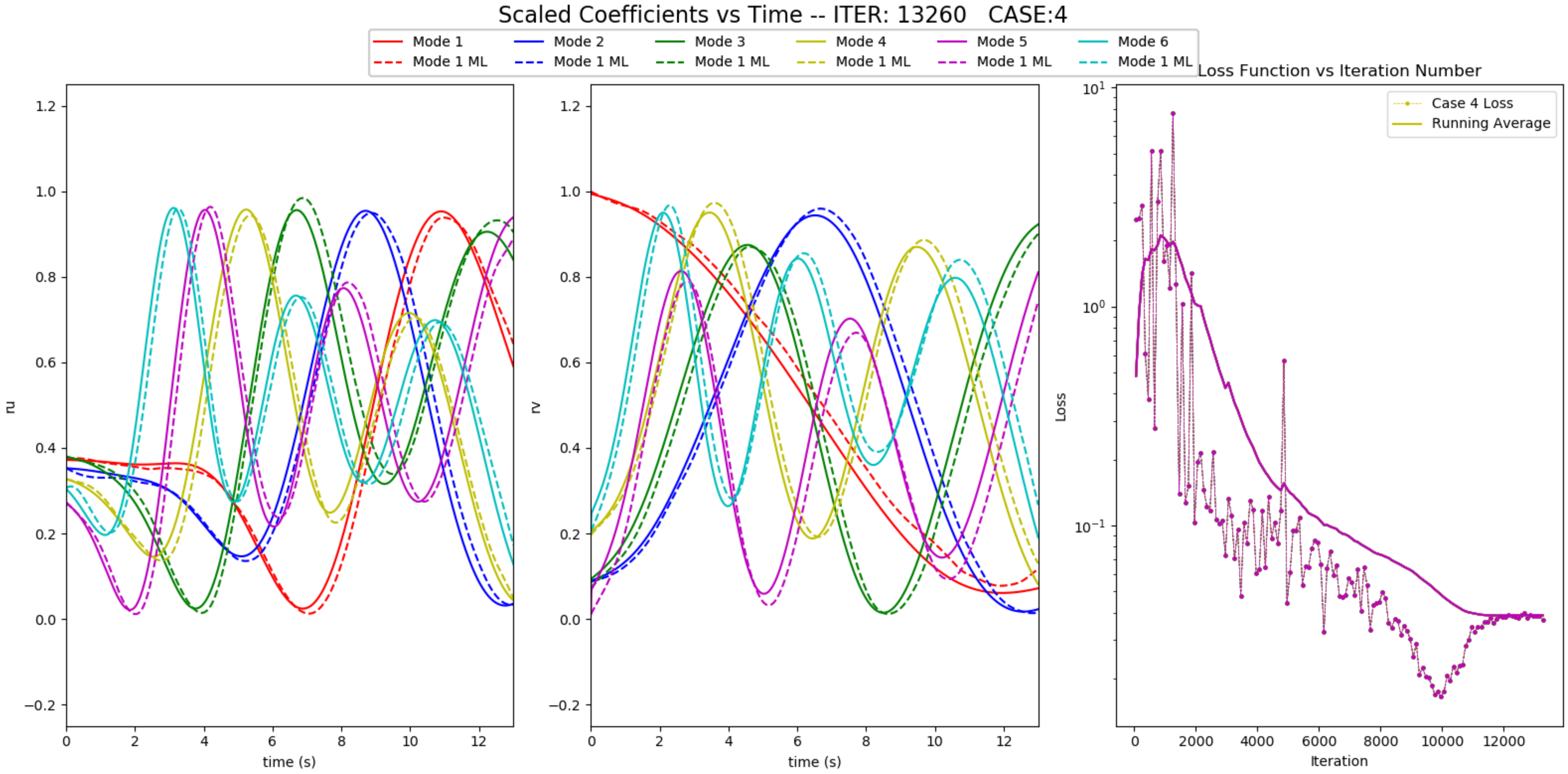
ML vs POD, Case 2, 13 seconds



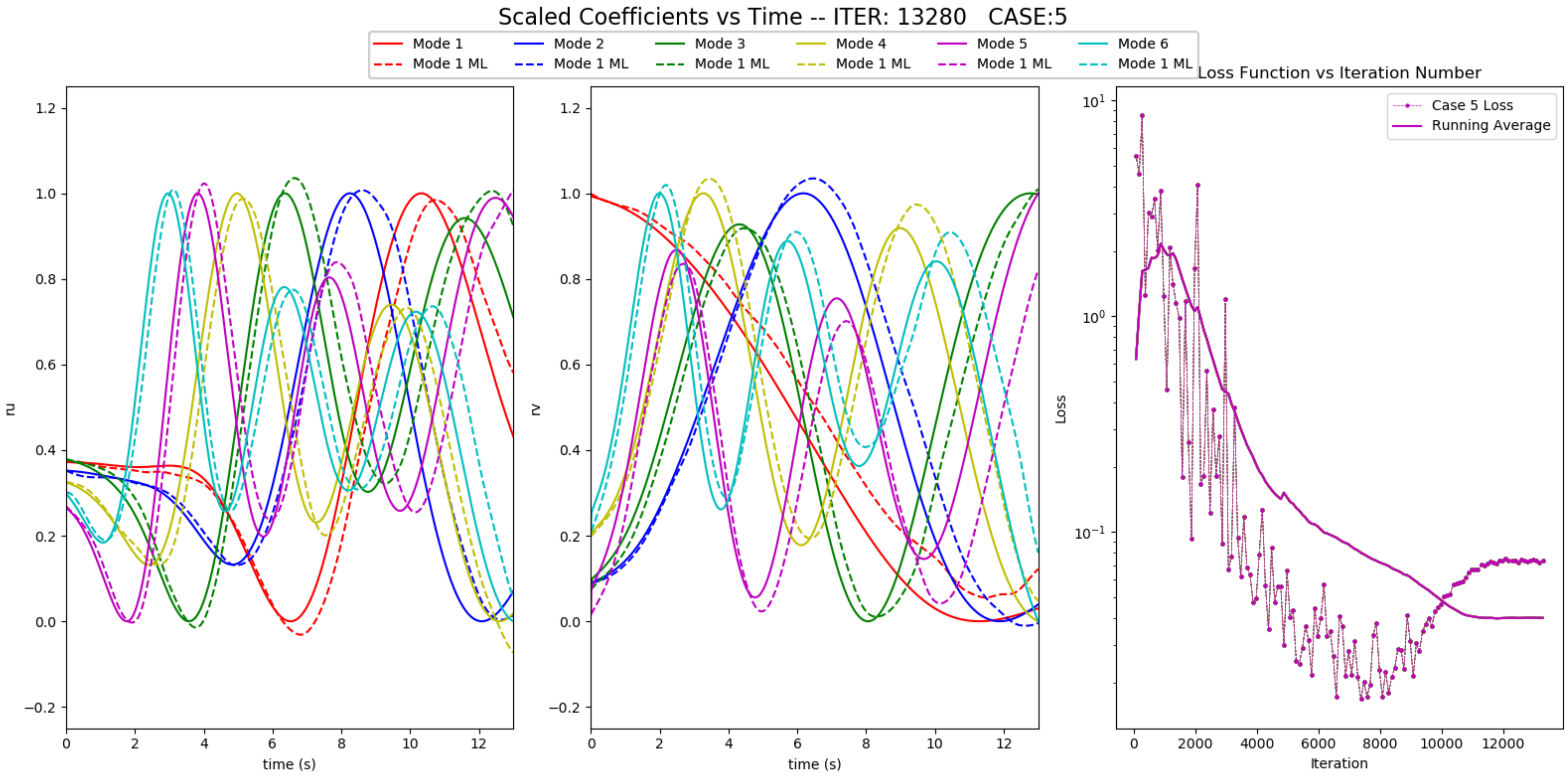
ML vs POD, Case 3, 13 seconds



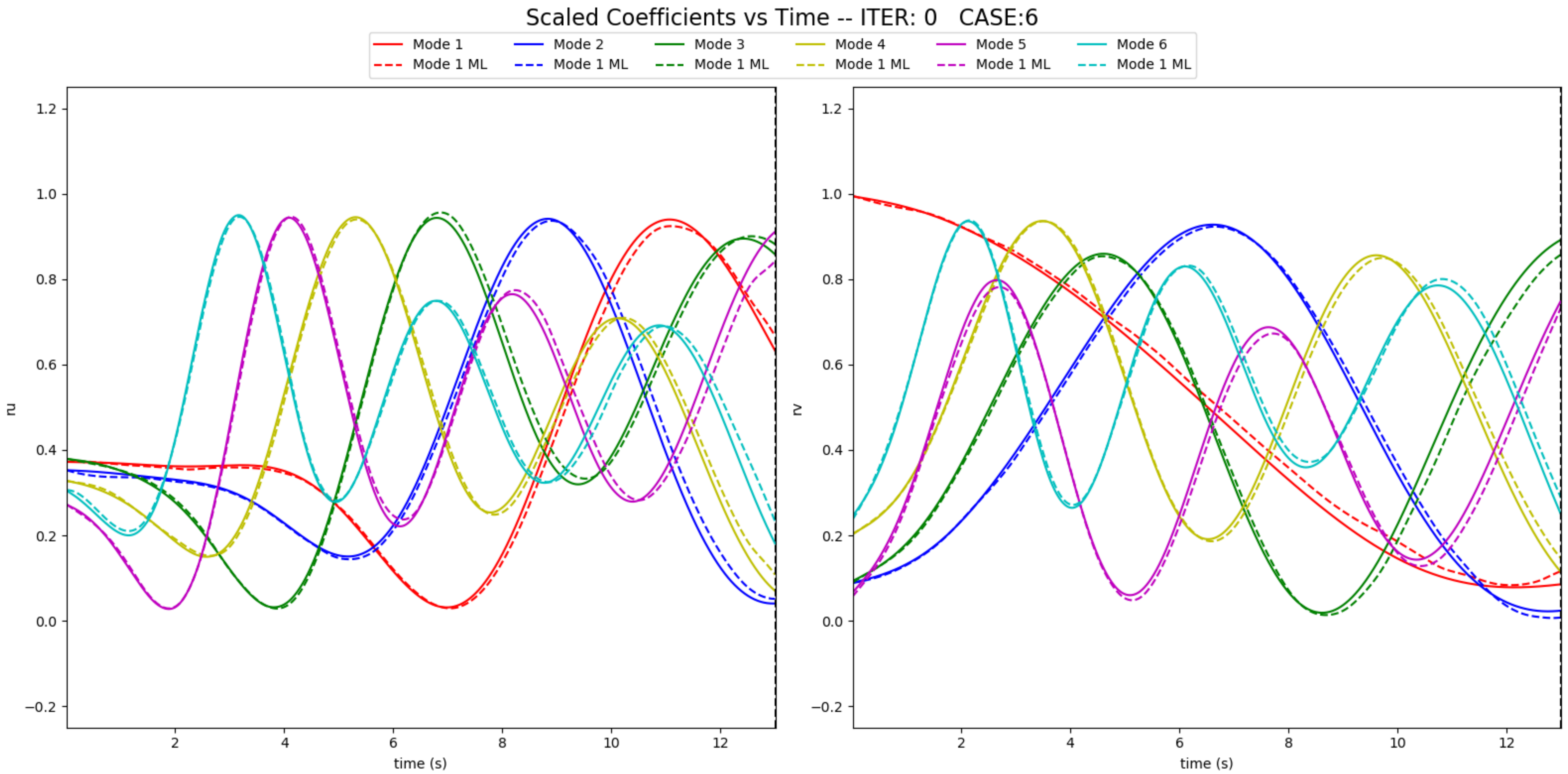
ML vs POD, Case 4, 13 seconds



ML vs POD, Case 5, 13 seconds



ML vs POD, Case 6, 13 seconds



Gas-Solids Dynamics in Fluidized Bed

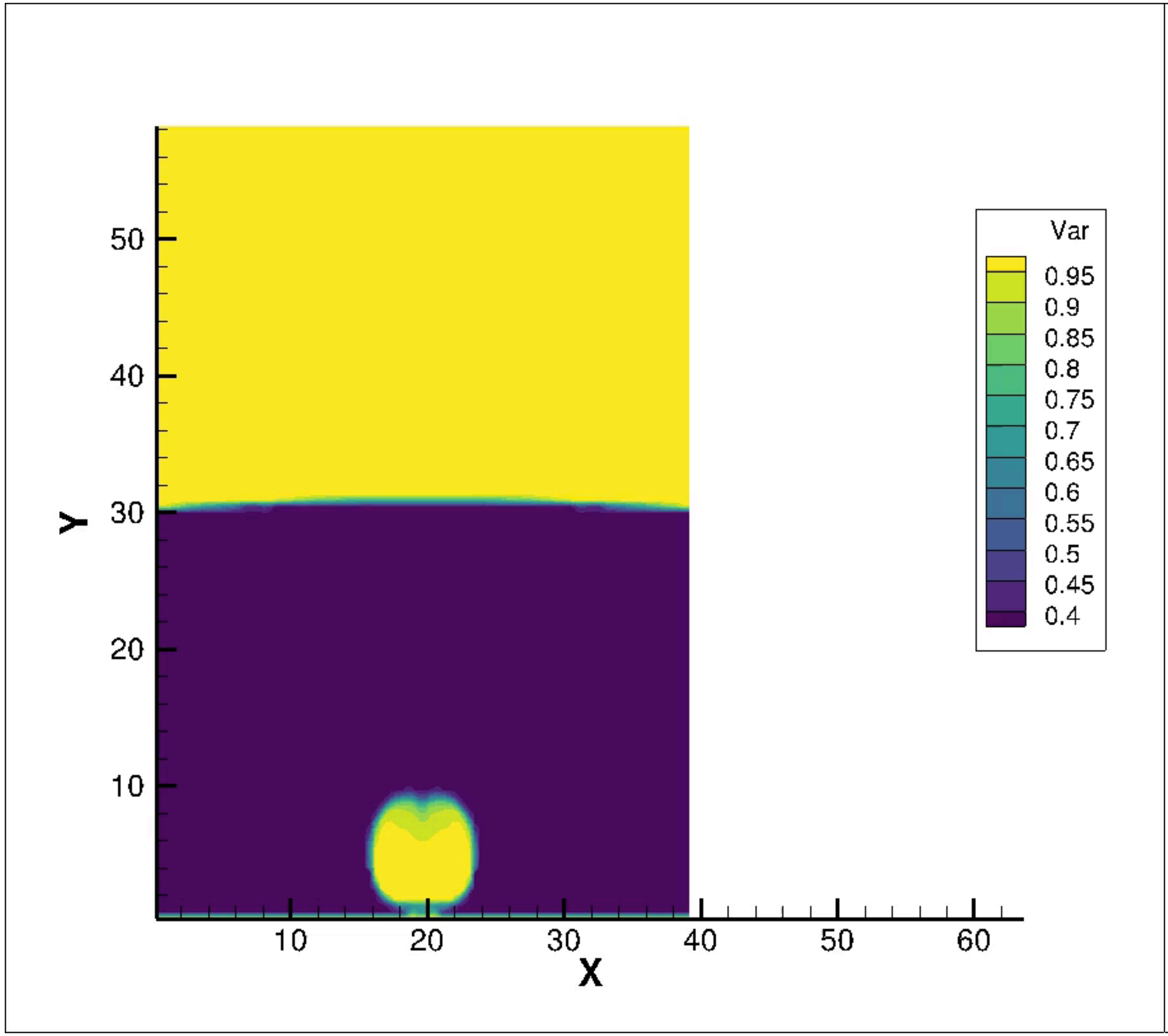
Variable Solids Density, RO_s

- Seven values for solids density - nominal density (2.61)

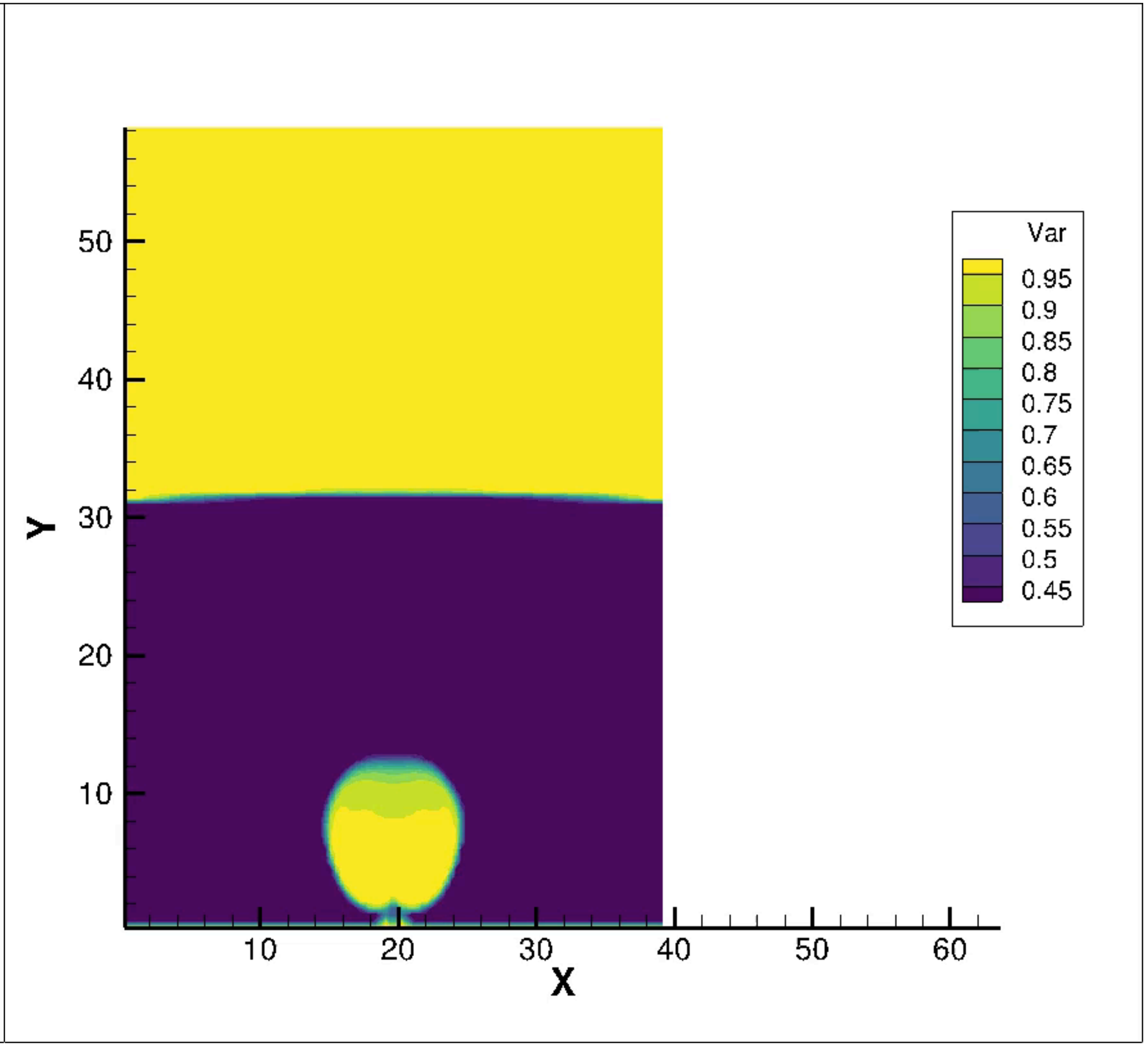
Case	Density Multiplier	
1	1	On
2	1.05	On
3	0.95	On
4	1.1	On
5	0.9	On
6	1.025	Off
7	0.975	Off

D. Gidaspow, Multiphase Flow and Fluidization (1994); M. Syamlal, “Higher Order Discretization Methods for the Numerical Simulation of Fluidized Beds”, AIChE Annual Meeting (1997)

Void Fraction



RO_g = 1.1 nominal

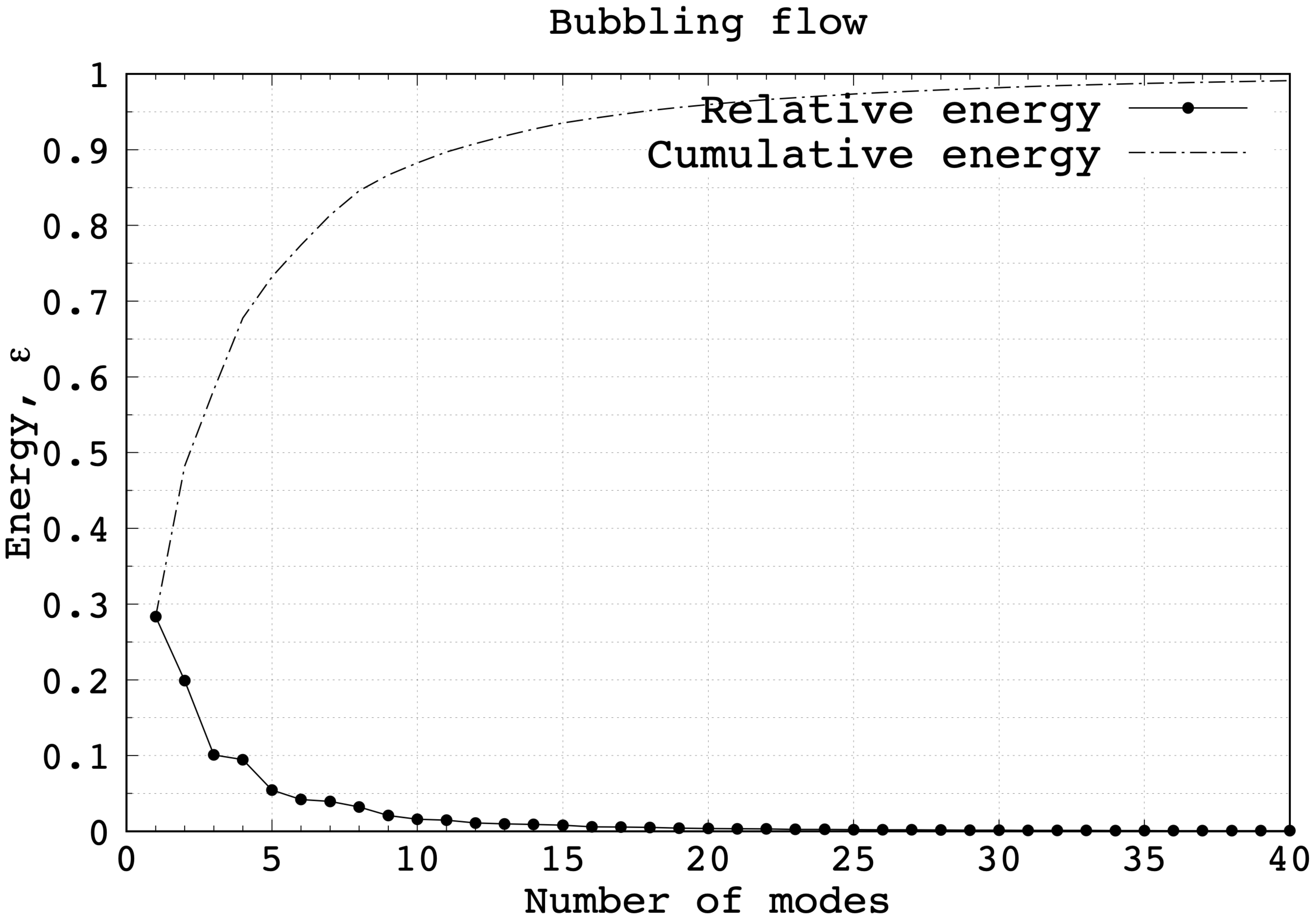


RO_g = 0.9 nominal

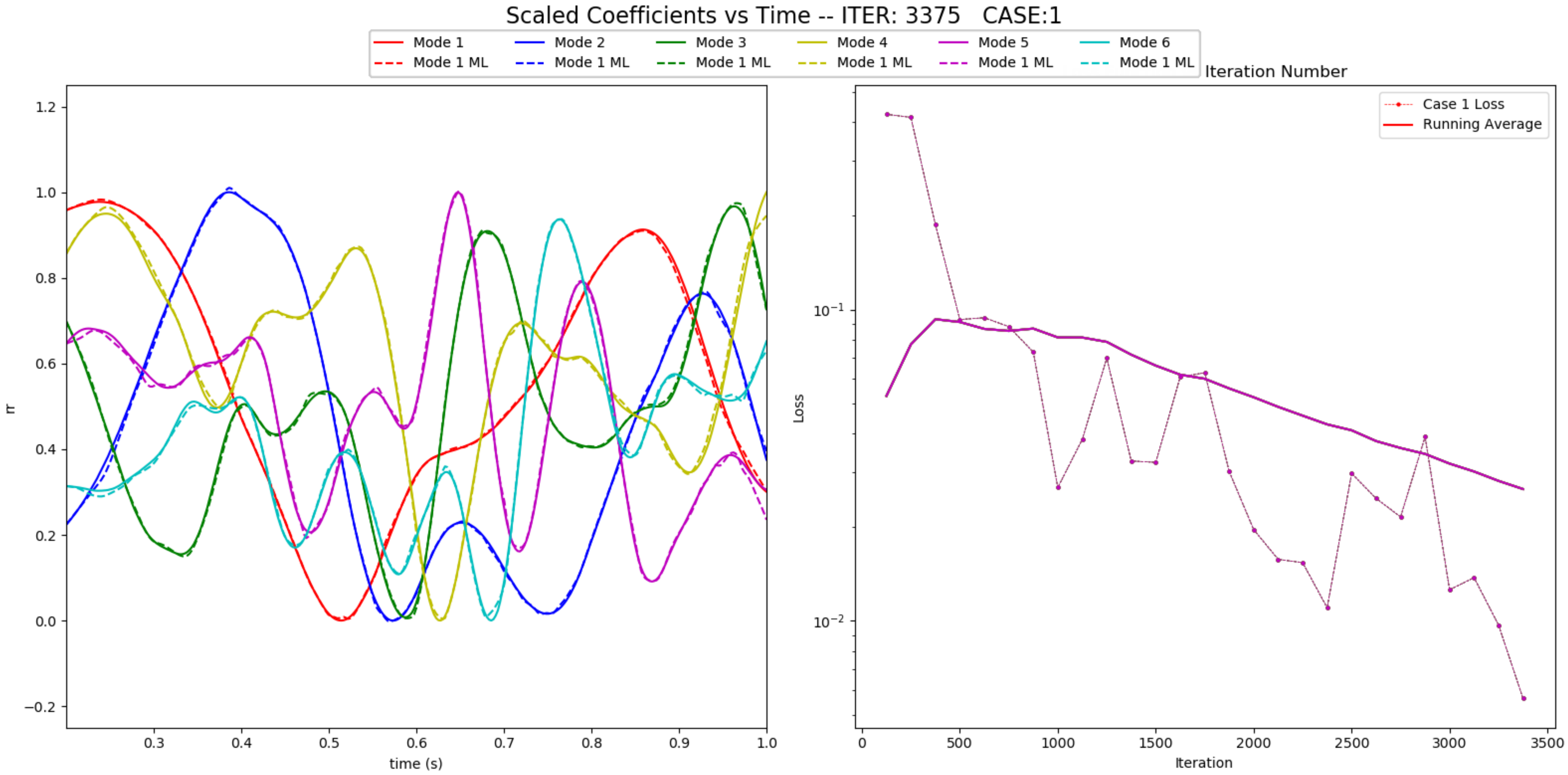
Bubbling Flow Modes

Modes

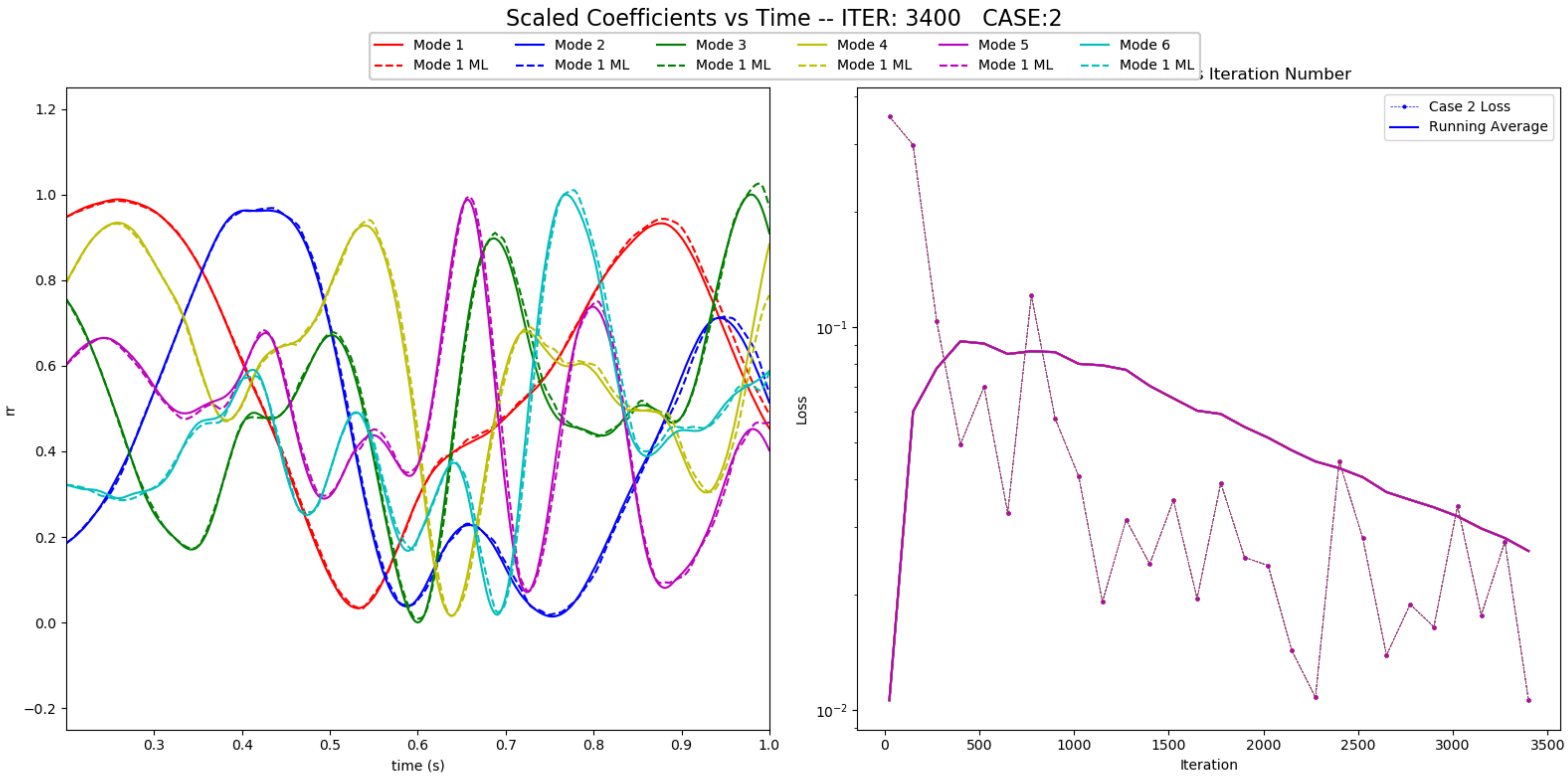
0 1 2 3 4


Bubbling flow
Relative energy
Cumulative energy
Energy, ε
Number of modes
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
5
10
15
20
25
30
35
40

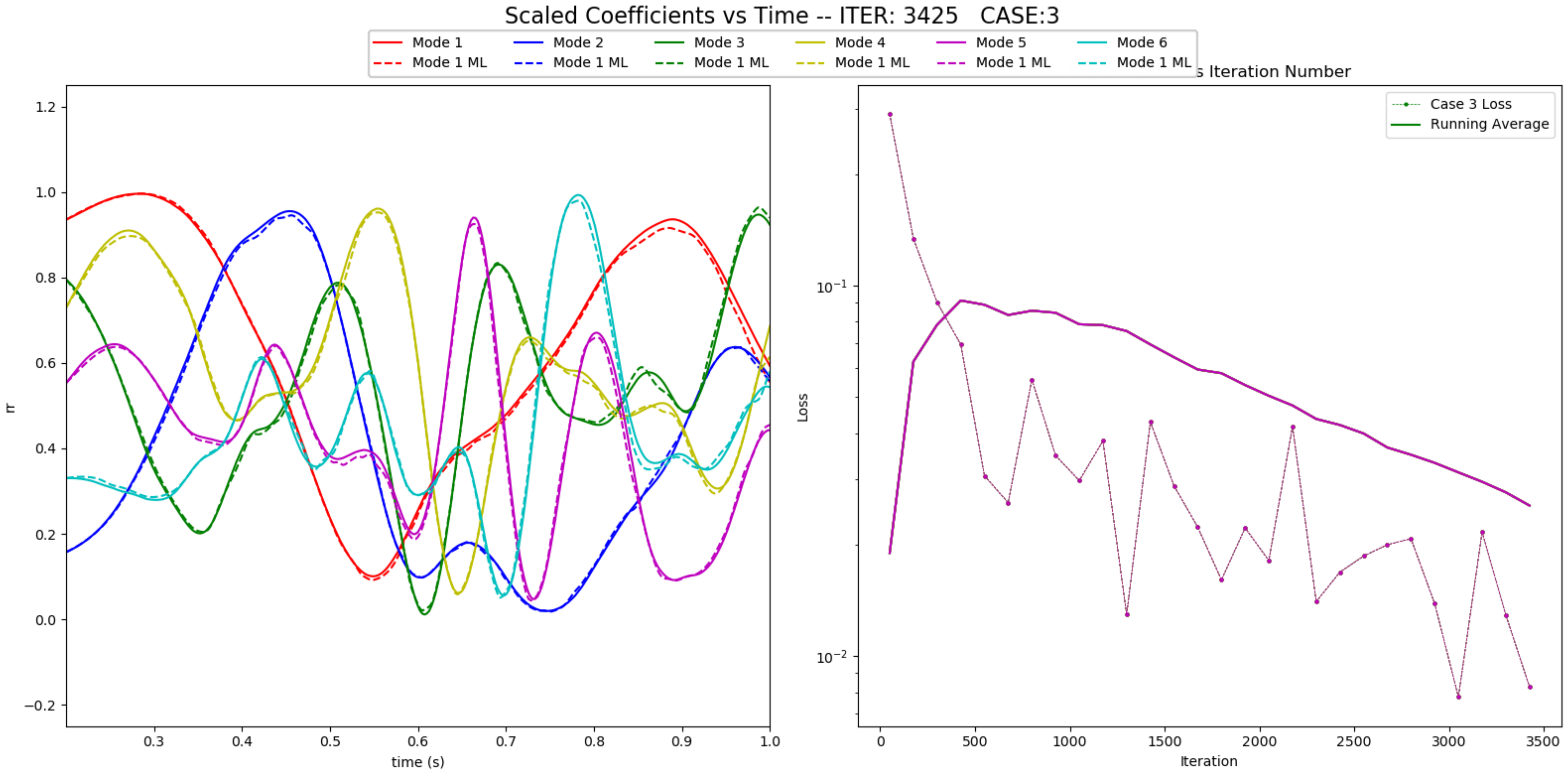
ML vs POD, Case 1, 1 second



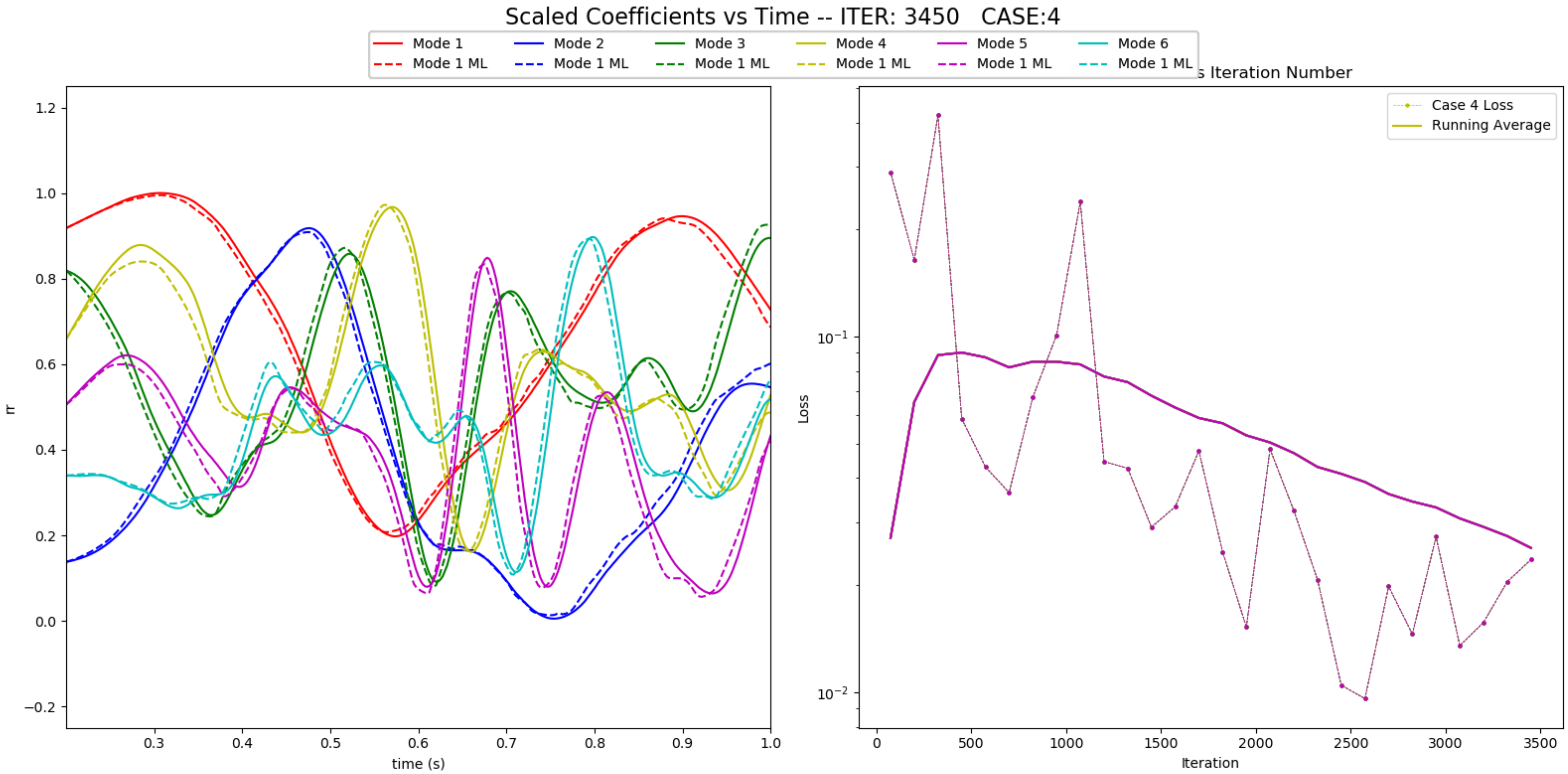
ML vs POD, Case 2, 1 second



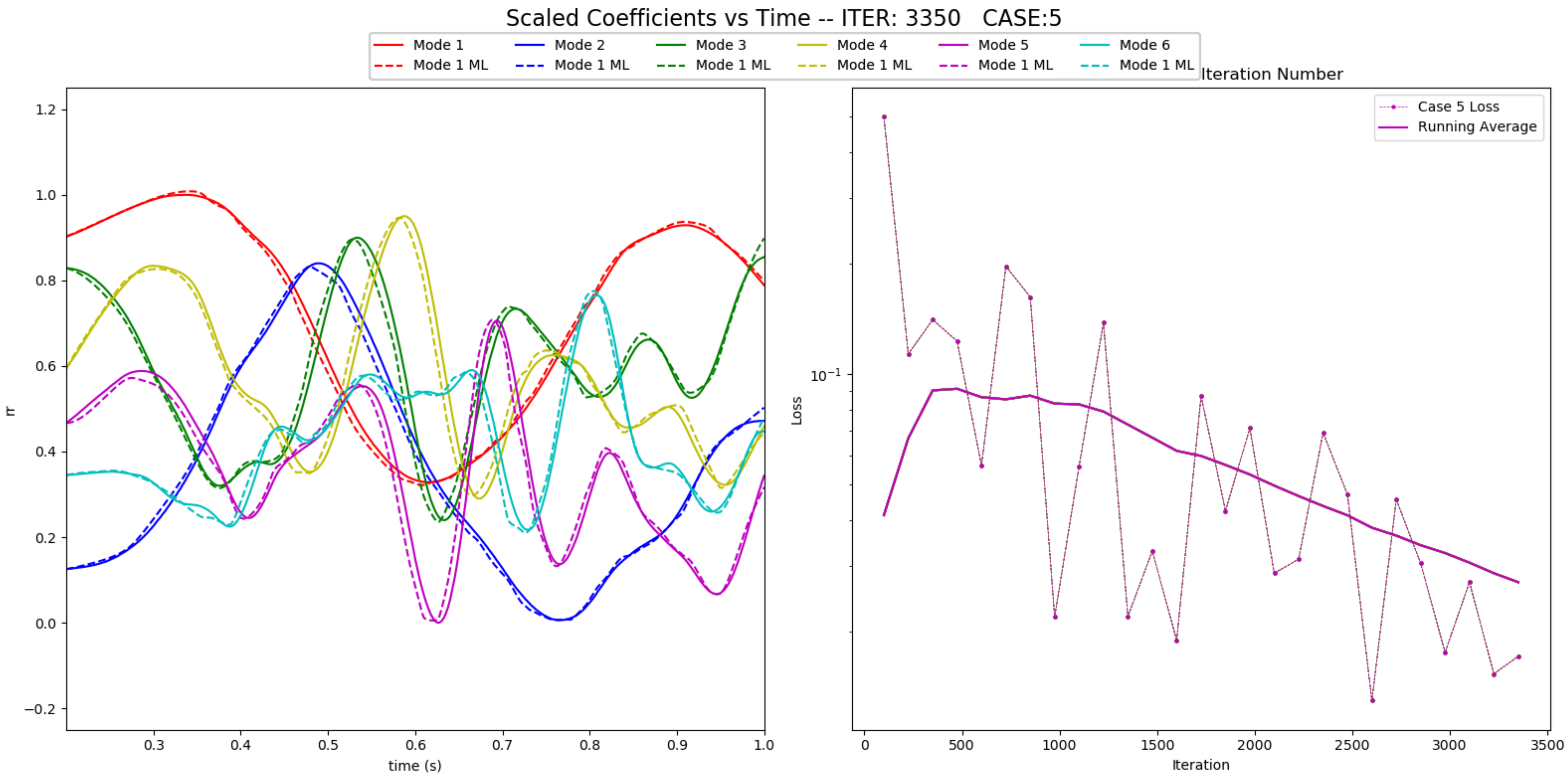
ML vs POD, Case 3, 1 second



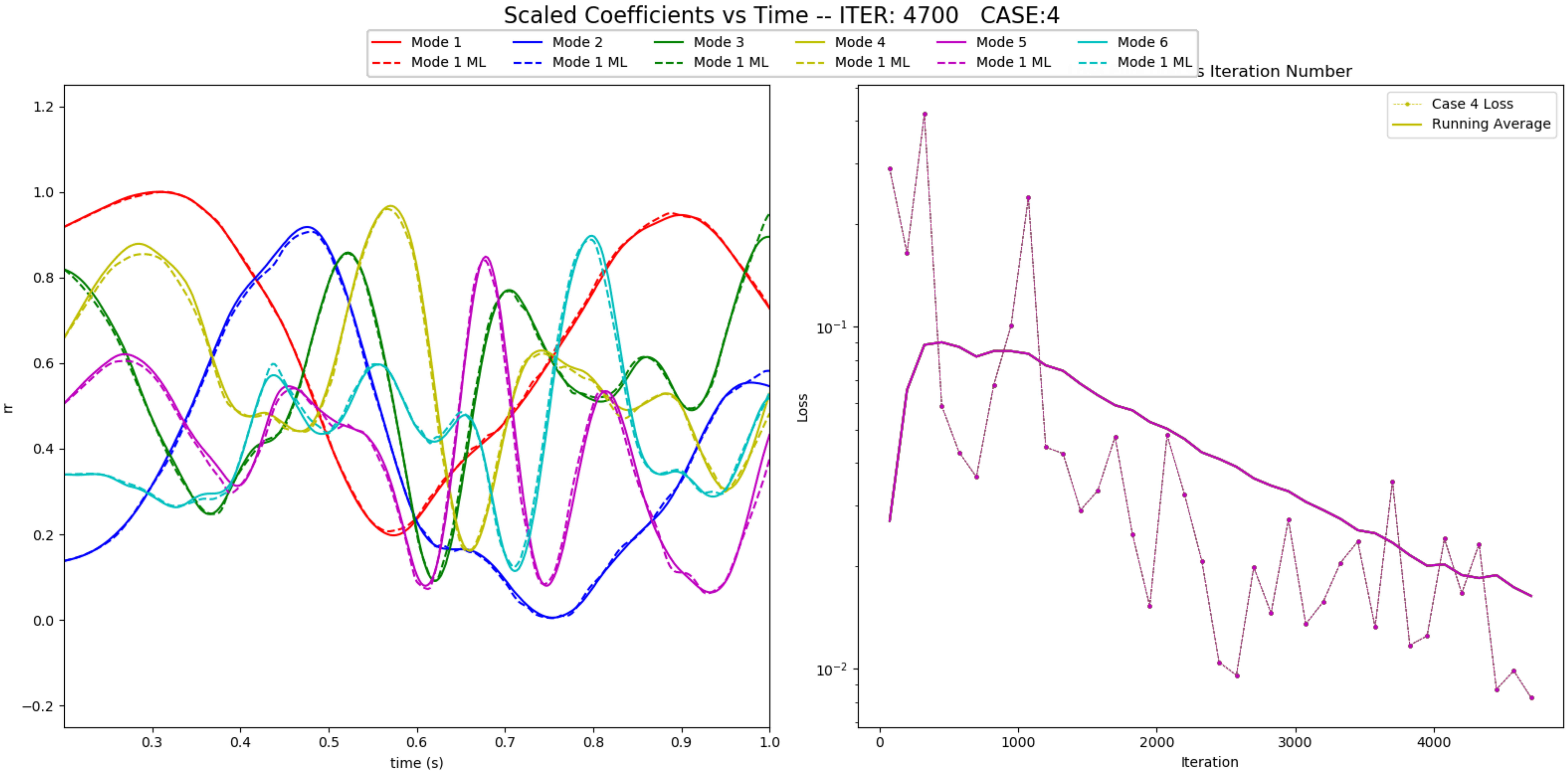
ML vs POD, Case 4, 1 second



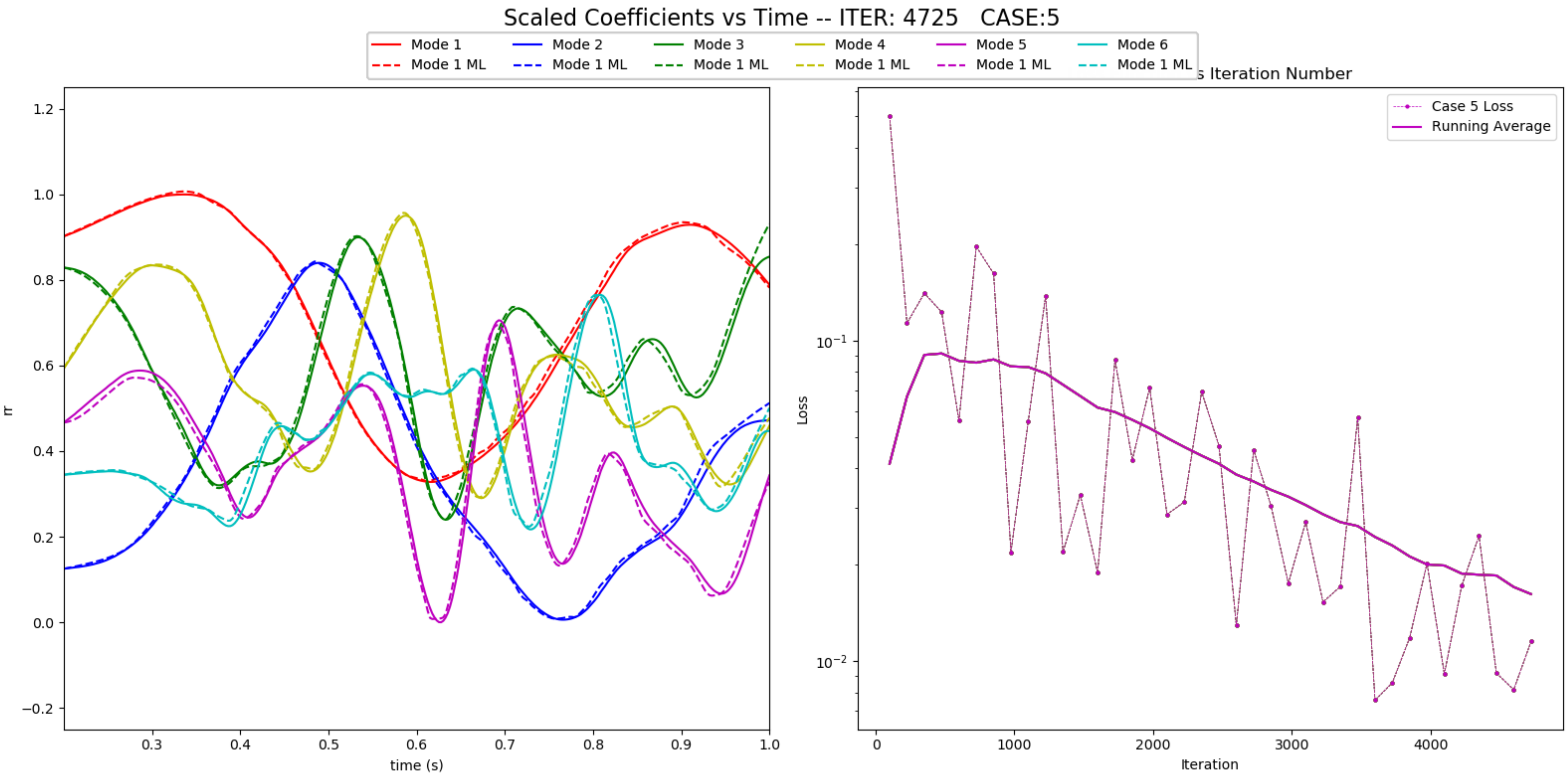
ML vs POD, Case 5, 1 second



ML vs POD, Case 6, 1 second



ML vs POD, Case 7, 1 second



Conclusions

- ML properly captured flow features of the three cases tested herein