Calculation of Invariant Manifolds for Reacting Systems

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Introduction

Motivation and background

- Reactive flow systems are multi-scale problems,
- severe stiffness arises in detailed gas-phase chemical kinetics modeling,
- detailed kinetics are essential for accurate modeling,
- computational cost for reactive flow simulations increases with the spatio-temporal scales' range, the number of species, and the number of reactions,
- manifold methods provide a potential for computational saving.

Partial Review of Manifold Methods in Reactive Systems

- The ILDM, CSP, and ICE-PIC are approximations of the reaction slow invariant manifold.
- MEPT and similar methods: based on the minimum thermodynamics potential function.
- IE method: requires reasonable initial conditions.
- Davis and Skodje, 1999: present a technique to construct the SIM based on global phase analysis.
- Creta *et al.* and Giona *et al.*, 2006: show the existence and uniqueness of the global SIM.

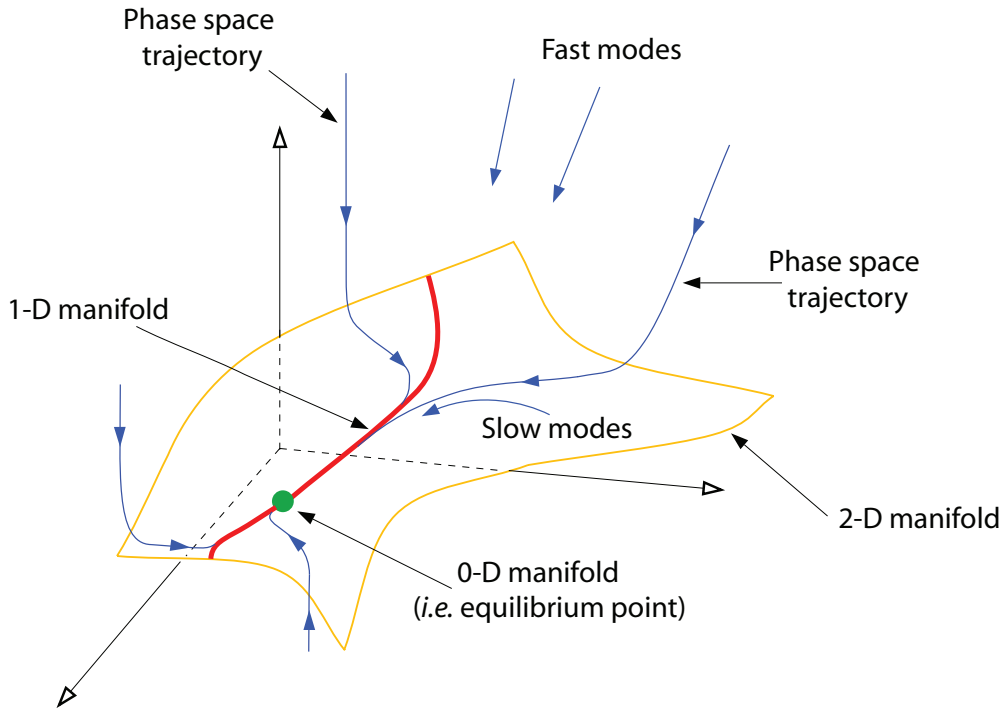
Objective

Create an efficient algorithm that reduces the computational cost for simulating a reactive flow system based on a reduction in the stiffness and dimension of the phase space $\mathbb{R}^N$.

Slow Invariant Manifold (SIM)

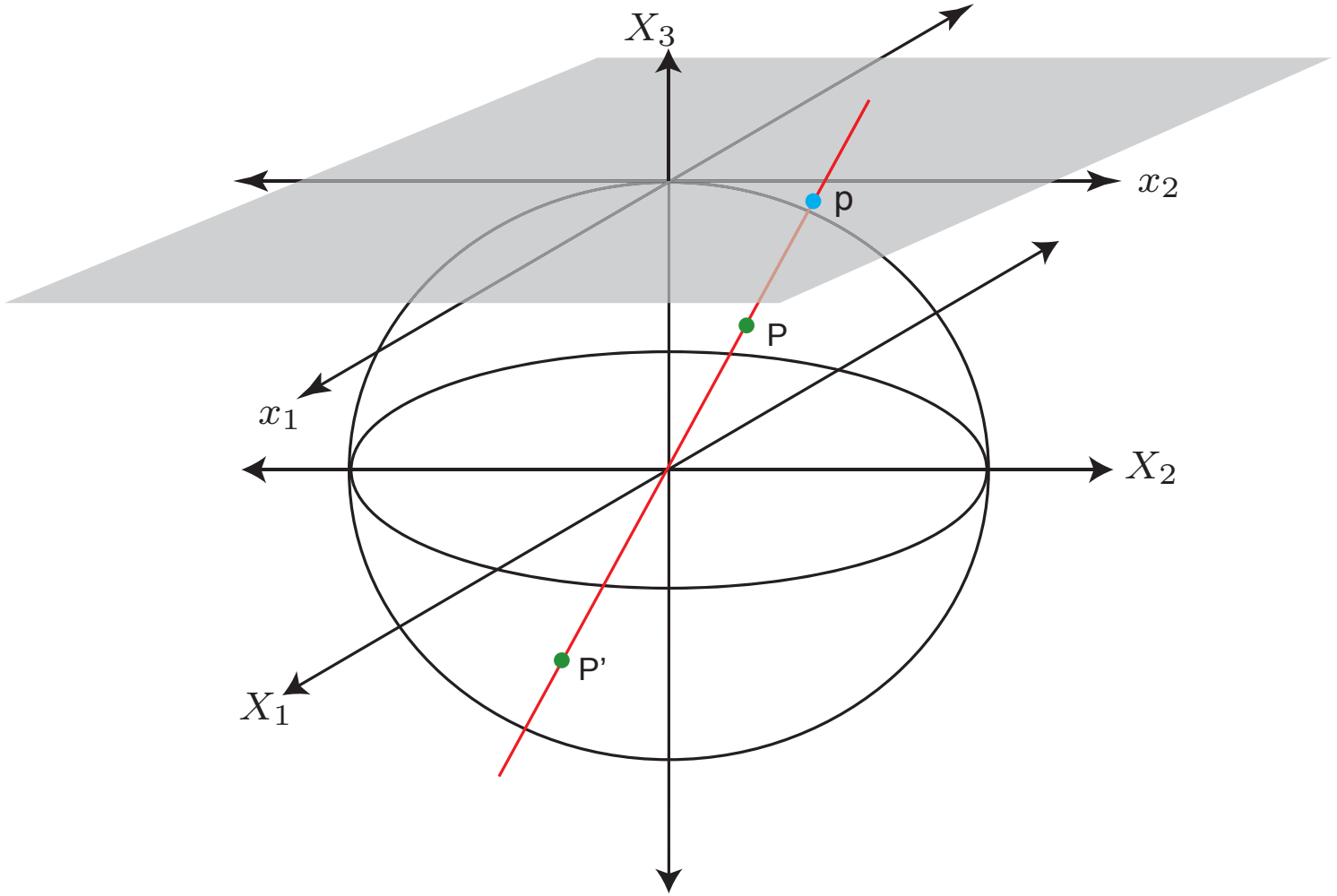
- The composition phase space for spatially homogeneous reactive system:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^N.$$



- An invariant manifold is defined as a subset $\mathcal{S} \subset \mathbb{R}^N$ if for any solution $\mathbf{x}(t)$, $\mathbf{x}(t_o) \in \mathcal{S}$, implies that for some $t_f > t_o$, $\mathbf{x}(t) \in \mathcal{S}$ for all $t \in [t_o, t_f]$,
- not all invariant manifolds are attracting,
- attractiveness of SIMs increases as the stiffness increases,
- on the SIM, only slow modes contribute,
- the SIMs can be constructed by identifying all critical points, finite and infinite, and connecting them via trajectories.

Poincaré Sphere



- Poincaré phase space mapping, $\mathbb{R}^N \longrightarrow \mathbb{R}^{N+1}$:

$$\begin{aligned} X_i &= \frac{x_i}{\sqrt{1+\sum_i x_i^2}}, \quad i=1,\ldots,N, \\ X_{N+1} &= \frac{1}{\sqrt{1+\sum_i x_i^2}}, \end{aligned}$$

- the infinite equilibria are the roots of the $G-$equations on the equator of Poincaré sphere:

$$G_k \equiv X_i\,\dot{X}_j(\mathbf{X}) - X_j\,\dot{X}_i(\mathbf{X}) = 0, \quad i,j=1,\ldots,N,\ i\neq j,\ k=1,\ldots,N-1$$

- to analyze the dynamical behavior, the flow has to be projected onto a plane tangent to the Poincaré sphere,

- for $N > 3$ it is computationally inefficient and algorithmically complex.

Alternative: Using Projective Space

- One-to-one mapping of the phase space, $\mathbb{R}^N \to \mathbb{R}^N$,

$$\begin{aligned} X_N &= \frac{1}{x_1}, \\ X_i &= \frac{x_k}{x_1}, \quad i = 1, \ldots, N-1, \quad k = 2, \ldots, N, \end{aligned}$$

- the equilibria are found in terms of ratios between the dependent variables,
- the critical points of the resulting vector field represents the finite and the infinite equilibria of the original vector field,
- $X_N = 0$ represents the infinite equilibria.

Computational methodology

- Species evolution equations are polynomials,
- the dynamical behaviour of such polynomials are of algebraic-geometric nature,
- numerical algebraic geometry lies at the intersection of algebraic geometry and numerical analysis[a],
- `Bertini`, a free software for computation in numerical algebraic geometry, will be used for computing the critical points.

[a] A. Sommese and C. Wampler, *The Numerical Solution of Systems of Polynomials,* World Science, 2005.

Simple Hydrogen System

- A kinetic model adopted from Michael J. V., 1992, *Prog. Energy Combust. Sci.*, **18** (4), pp. 327-345,
- the mechanism consist of $J = 8$ elementary bimolecular reactions involving $L = 2$ elements, and $N = 6$ species, H_2, O_2, H, O, OH, and H_2O,
- spatially homogenous with isothermal and isochoric conditions, $T = 1000\ K, p_o = 0.5\ atm$,
- the system evolution ODEs are recast as DAEs.

DAEs formulation

$$\frac{d}{dt}\begin{pmatrix} \bar{\rho}_{H_2} \\ \bar{\rho}_O \\ \bar{\rho}_{O_2} \end{pmatrix} = \begin{pmatrix} \dot{\omega}_{H_2} \\ \dot{\omega}_O \\ \dot{\omega}_{O_2} \end{pmatrix} \equiv \mathbf{h},$$

$$\begin{aligned}
\bar{\rho}_O + \bar{\rho}_{OH} + \bar{\rho}_{H_2O} + 2\bar{\rho}_{O_2} &= [\bar{\rho}_O + \bar{\rho}_{OH} \\
&\quad +\bar{\rho}_{H_2O} + 2\bar{\rho}_{O_2}]_o\,, \\
\bar{\rho}_H + \bar{\rho}_{OH} + 2\bar{\rho}_{H_2O} + 2\bar{\rho}_{H_2} &= [\bar{\rho}_H + \bar{\rho}_{OH} \\
&\quad +2\bar{\rho}_{H_2O} + 2\bar{\rho}_{H_2}]_o\,, \\
\bar{\rho}_H + \bar{\rho}_{H_2} + \bar{\rho}_{O_2} + \bar{\rho}_O + \bar{\rho}_{OH} + \bar{\rho}_{H_2O} &= [\bar{\rho}_H + \bar{\rho}_{H_2} + \bar{\rho}_{O_2} \\
&\quad +\bar{\rho}_O + \bar{\rho}_{OH} + \bar{\rho}_{H_2O}]_o\,,
\end{aligned}$$

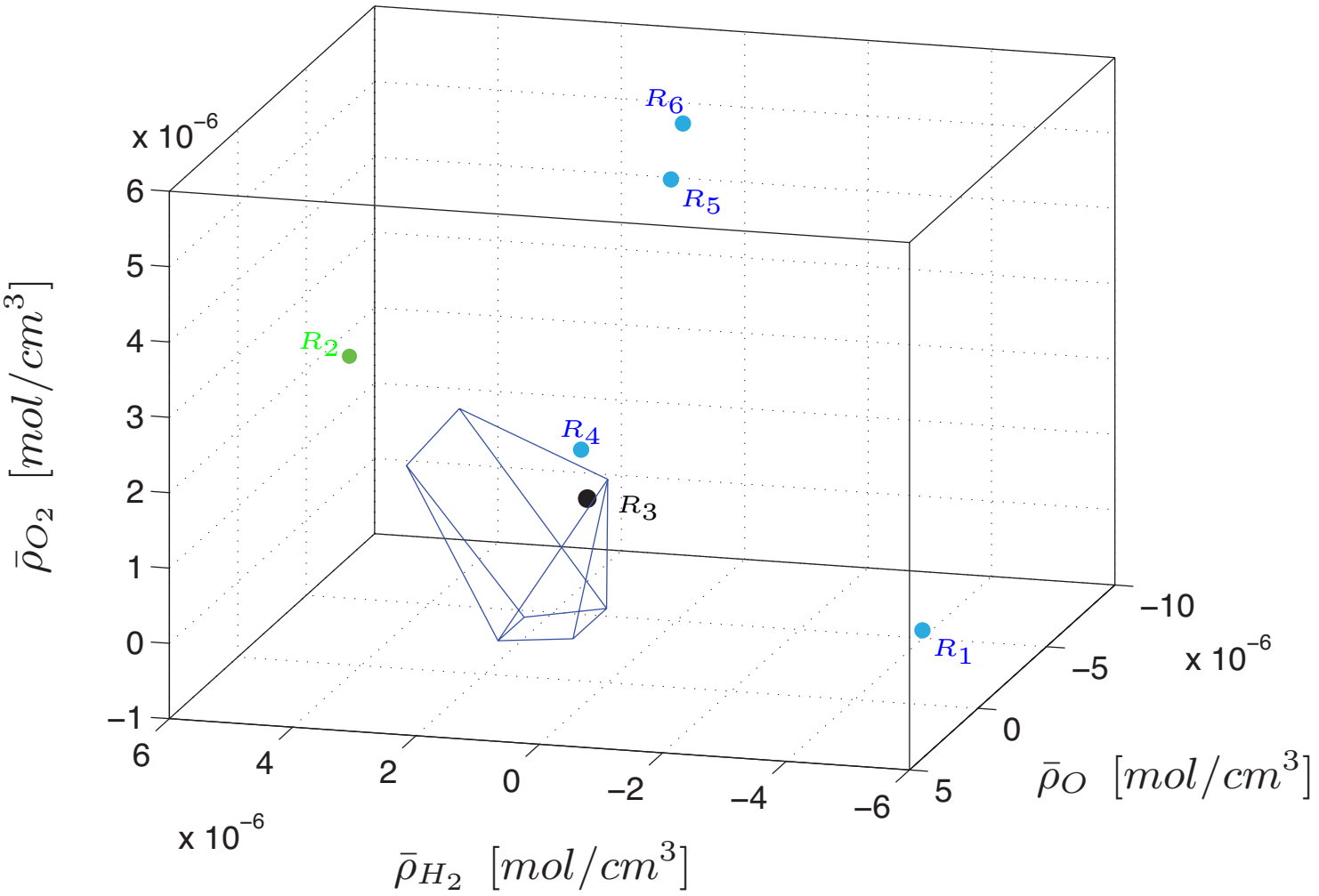
the $\bar{\rho}$ are given in units of mol/cm^3 and the $\dot{\omega}$ in units of $mol/cm^3/s$.

Dynamical system analysis

$$
\begin{aligned}
R_1 \equiv (\bar{\rho}^e_{H_2}, \bar{\rho}^e_O, \bar{\rho}^e_{O_2}) &= \left(-5.101 \times 10^{-6}, 2.021 \times 10^{-8}, -1.136 \times 10^{-8}\right), \\
(\lambda_1, \lambda_2, \lambda_3) &= (4.97996 \times 10^6, 1.57592 \times 10^6, -3.37824 \times 10^5), \\
R_2 \equiv (\bar{\rho}^e_{H_2}, \bar{\rho}^e_O, \bar{\rho}^e_{O_2}) &= \left(4.186 \times 10^{-6}, 0.0, 3.093 \times 10^{-6}\right), \\
(\lambda_1, \lambda_2, \lambda_3) &= (-5.88016 \times 10^6, -1.19776 \times 10^6, 2.55011 \times 10^5), \\
R_3 \equiv (\bar{\rho}^e_{H_2}, \bar{\rho}^e_O, \bar{\rho}^e_{O_2}) &= \left(2.411 \times 10^{-7}, 4.061 \times 10^{-7}, 1.495 \times 10^{-6}\right), \\
(\lambda_1, \lambda_2, \lambda_3) &= (-7.05241 \times 10^6, -3.31066 \times 10^5, -9.99734 \times 10^4), \\
R_4 \equiv (\bar{\rho}^e_{H_2}, \bar{\rho}^e_O, \bar{\rho}^e_{O_2}) &= \left(4.460 \times 10^{-7}, -6.543 \times 10^{-8}, 2.003 \times 10^{-6}\right), \\
(\lambda_1, \lambda_2, \lambda_3) &= (4.59069 \times 10^6, 1.75881 \times 10^6, 5.10102 \times 10^5), \\
R_5 \equiv (\bar{\rho}^e_{H_2}, \bar{\rho}^e_O, \bar{\rho}^e_{O_2}) &= \left(3.547 \times 10^{-8}, -4.764 \times 10^{-6}, 4.894 \times 10^{-6}\right), \\
(\lambda_1, \lambda_2, \lambda_3) &= (6.14154 \times 10^7, 1.10481 \times 10^6, -1.40938 \times 10^5), \\
R_6 \equiv (\bar{\rho}^e_{H_2}, \bar{\rho}^e_O, \bar{\rho}^e_{O_2}) &= \left(3.933 \times 10^{-8}, -5.660 \times 10^{-6}, 5.493 \times 10^{-6}\right), \\
(\lambda_1, \lambda_2, \lambda_3) &= (7.30643 \times 10^7, 1.30698 \times 10^6, 3.40968 \times 10^5),
\end{aligned}
$$

the $\bar{\rho}^{\,e}$ are given in units of mol/cm^3 and the λ in units of $1/s$.

Finite phase space



Results

- By employing the projective space mapping,

$$\frac{d}{d\tau}\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ t \end{pmatrix} = \begin{pmatrix} \dot{\Omega}_1 \\ \dot{\Omega}_2 \\ \dot{\Omega}_3 \\ X_3 \end{pmatrix} \equiv \mathbf{H},$$

  - the critical points of the vector space $\mathbf{H}$, which has $X_3 = 0$, represent the infinite equilibria of the vector space $\mathbf{h}$,
  - the critical points of the vector space $\mathbf{H}$, which has $X_3 \neq 0$, represent the finite equilibria of the vector space $\mathbf{h}$.

Dynamical system analysis

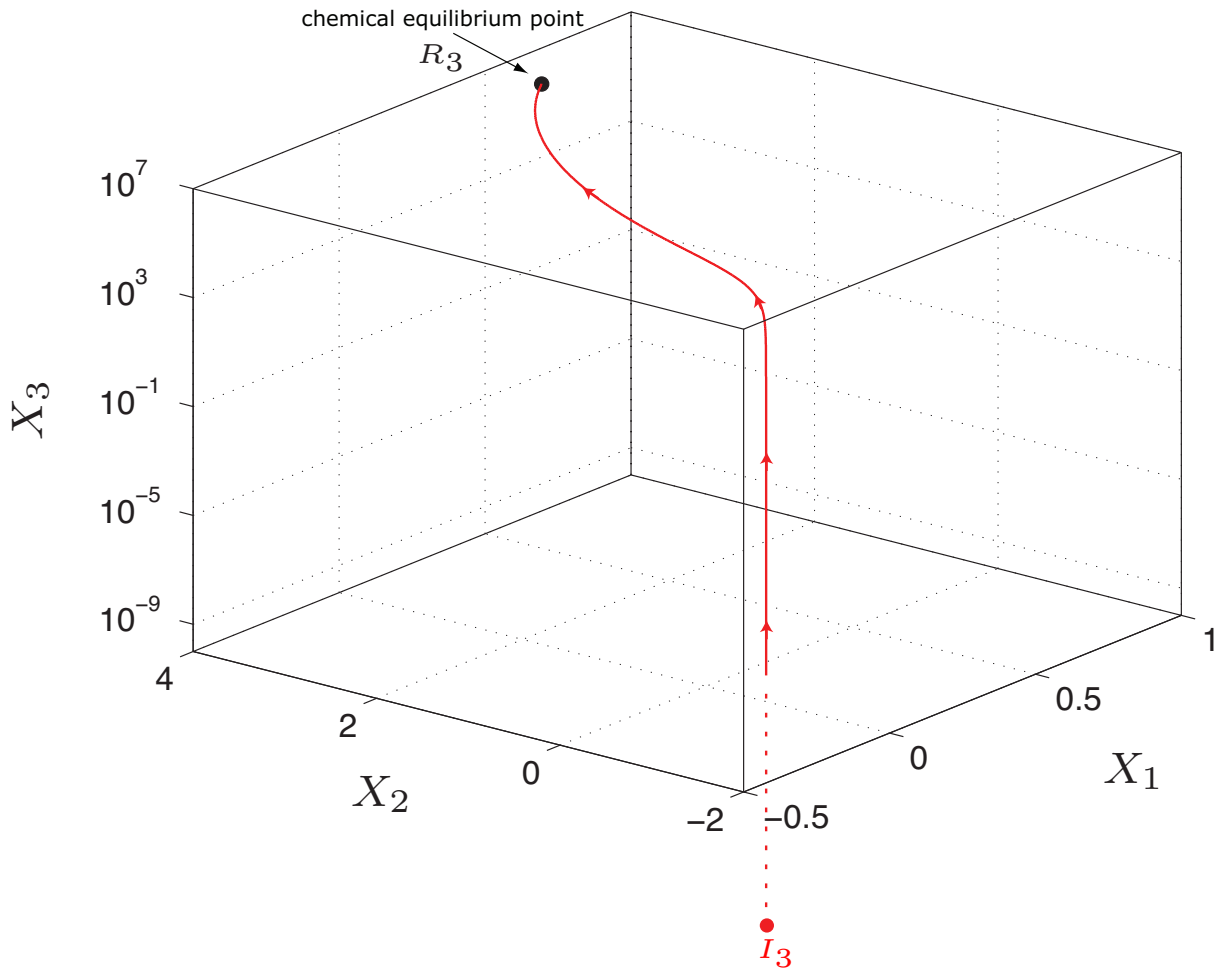
$$
\begin{aligned}
I_1(X_1, X_2, X_3) &= (-21.1206, -9.28413, 0.0), \\
(\lambda_1, \lambda_2, \lambda_3) &= (-2.99236 \times 10^{13} \pm 1.093 \times 10^{13} i, 7.40007 \times 10^{12}),
\end{aligned}
$$

$$
\begin{aligned}
I_2(X_1, X_2, X_3) &= (0.547525, -0.487801, 0.0), \\
(\lambda_1, \lambda_2, \lambda_3) &= (-1.34892 \times 10^{13}, 2.39079 \times 10^{11}, 2.20957 \times 10^{11}),
\end{aligned}
$$

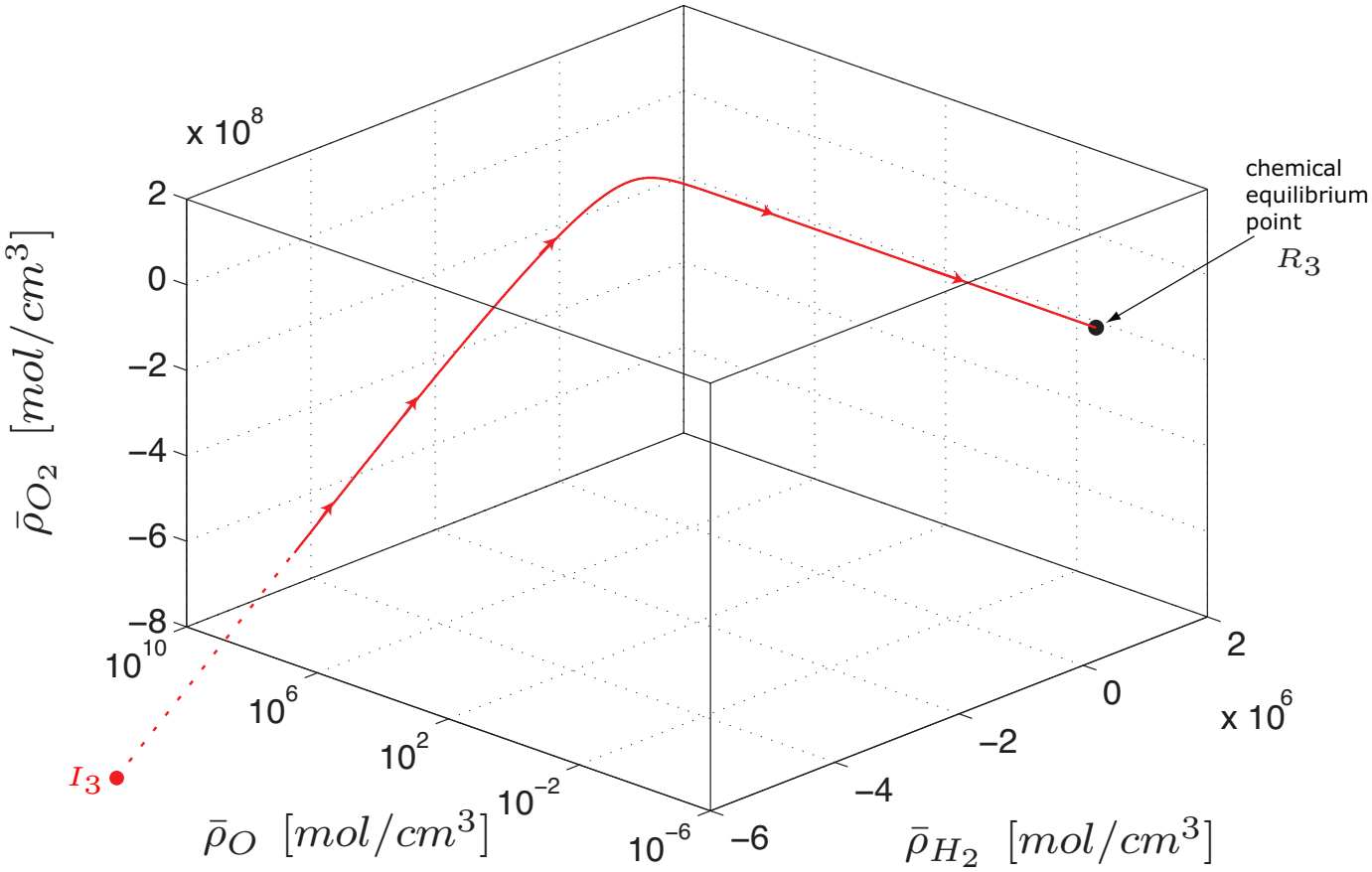
$$
\begin{aligned}
I_3(X_1, X_2, X_3) &= (-0.00479484, -0.668911, 0.0), \\
(\lambda_1, \lambda_2, \lambda_3) &= (-1.30206 \times 10^{13}, -2.24731 \times 10^{11}, 1.581 \times 10^{9}),
\end{aligned}
$$

- the critical point I_3 in the unstable direction is 2 orders of magnitude smaller than the rest of the eigenvalues,
- small eigenvalue $\equiv$ slow mode, $\tau = 1/\left|Re[\lambda]\right|$.

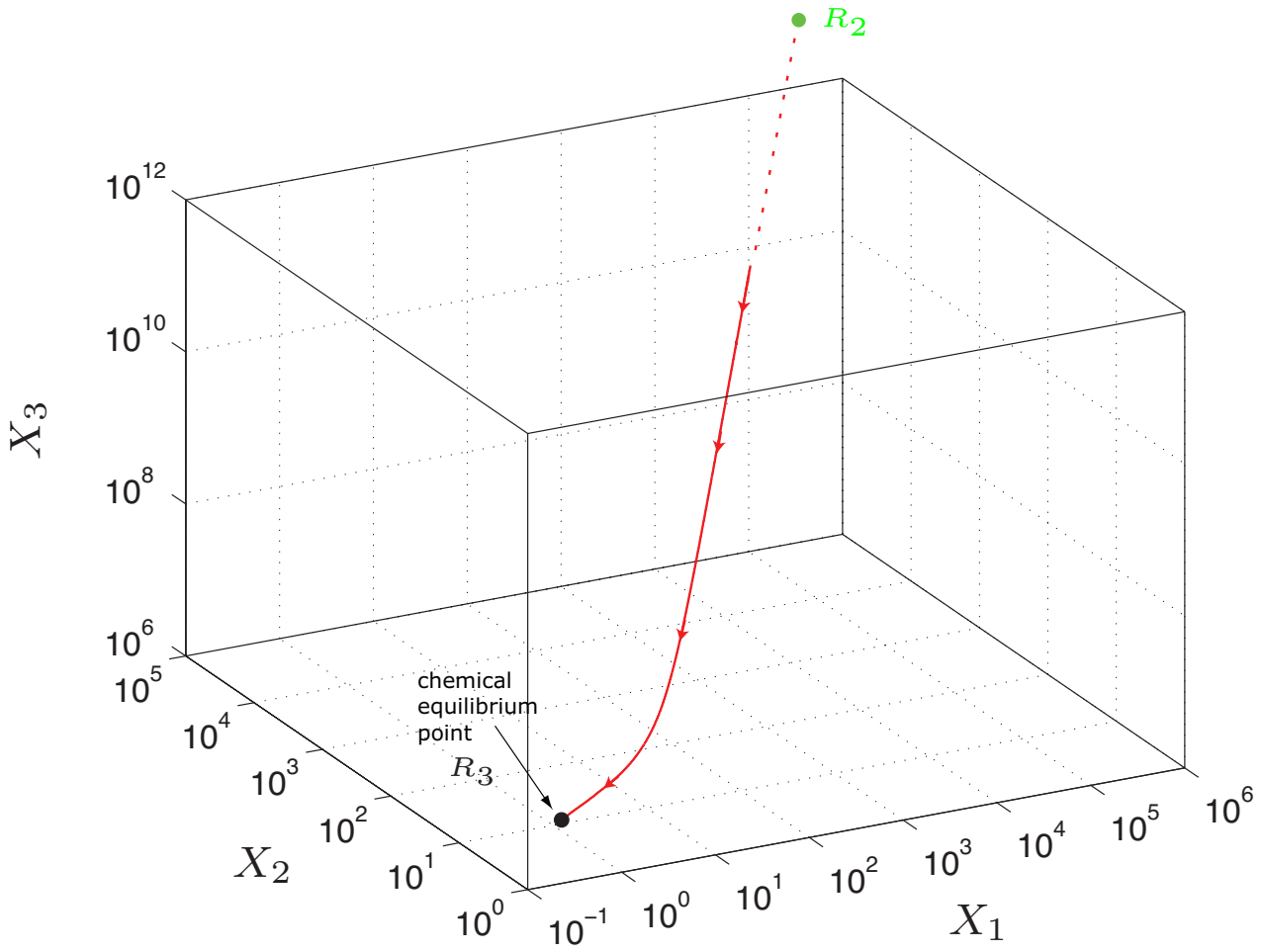
- By integrating from I_3,



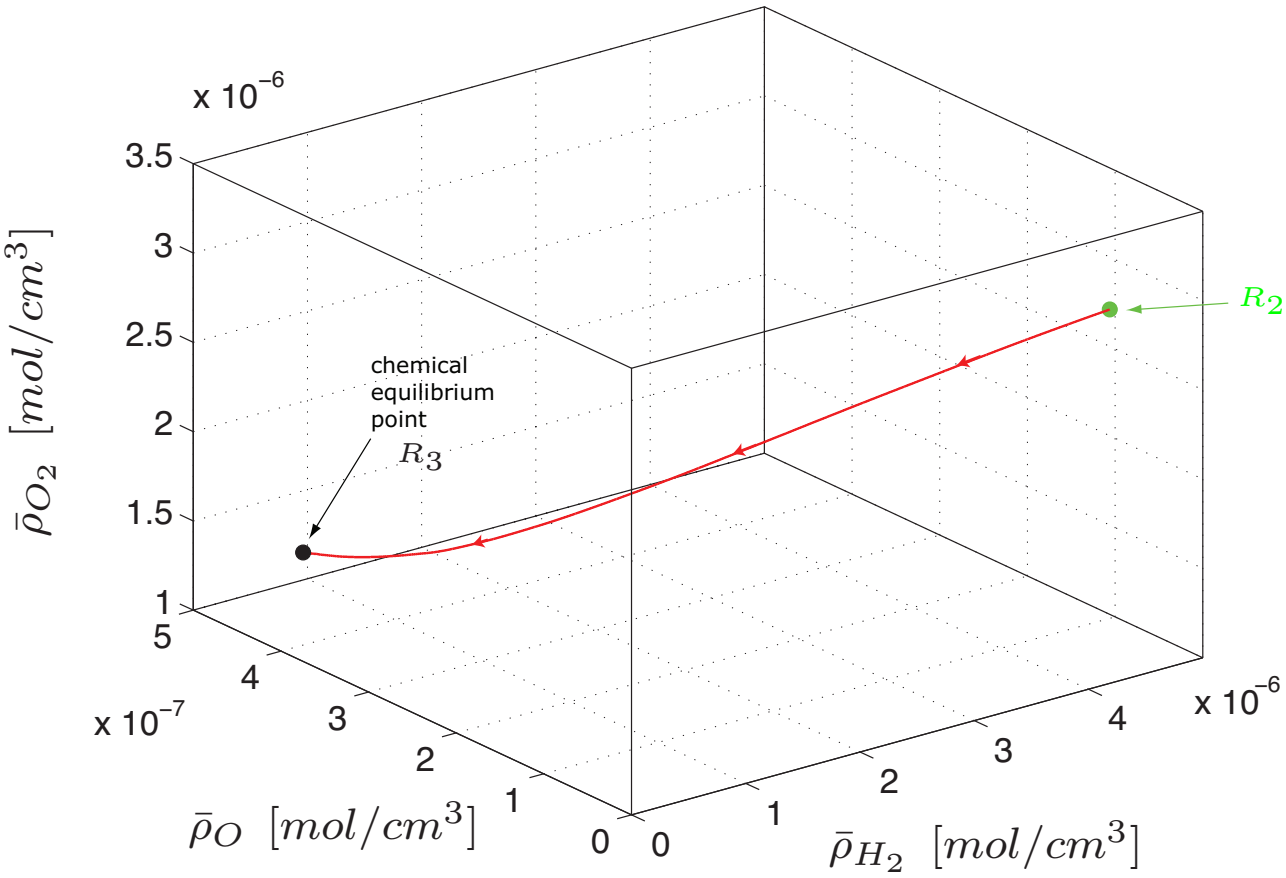
- Mapping the SIM into the original $\mathbb{R}^3$,



- The second branch of the SIM in the projective space,

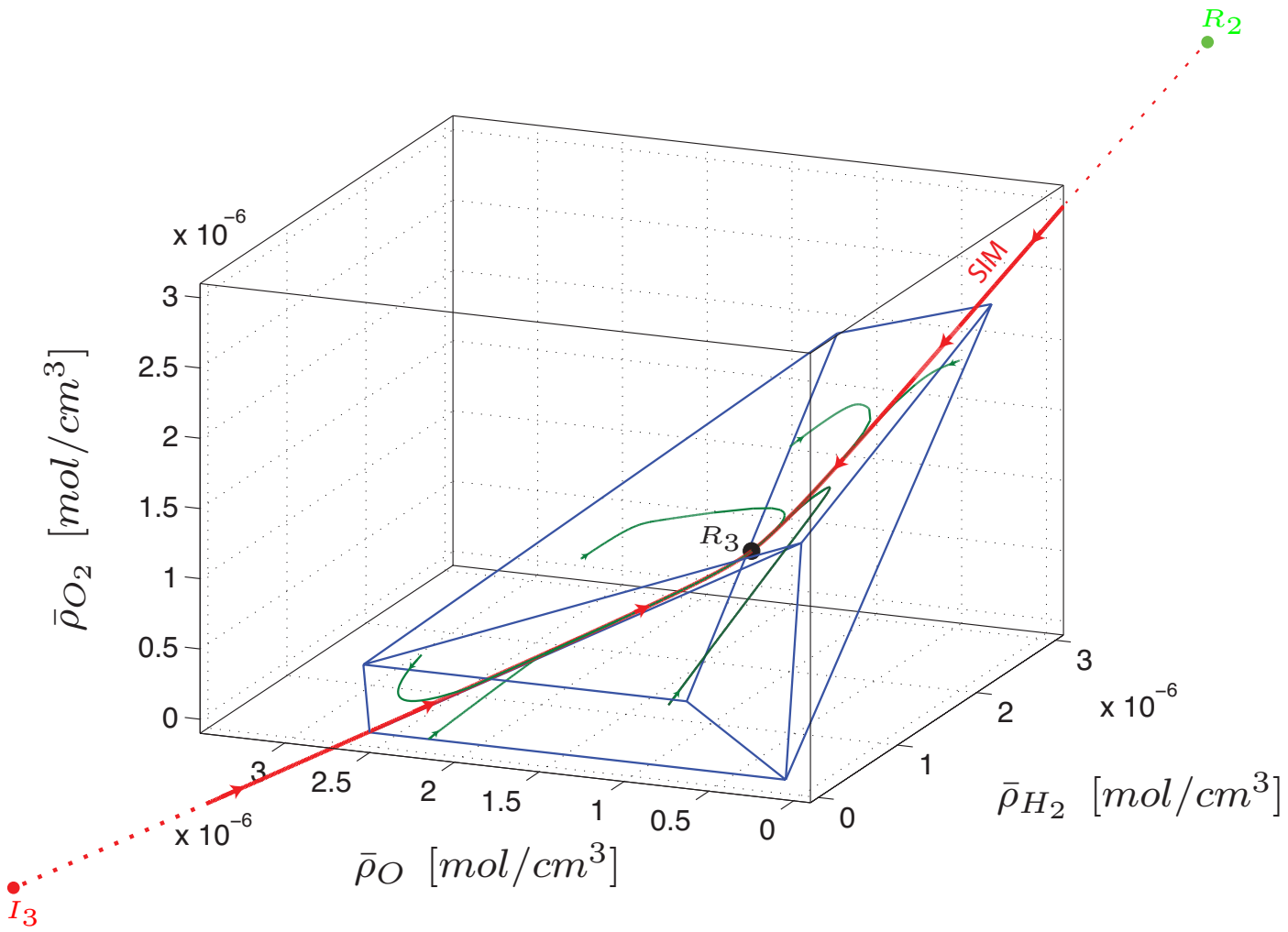


- The second branch mapped into the original $\mathbb{R}^3$,



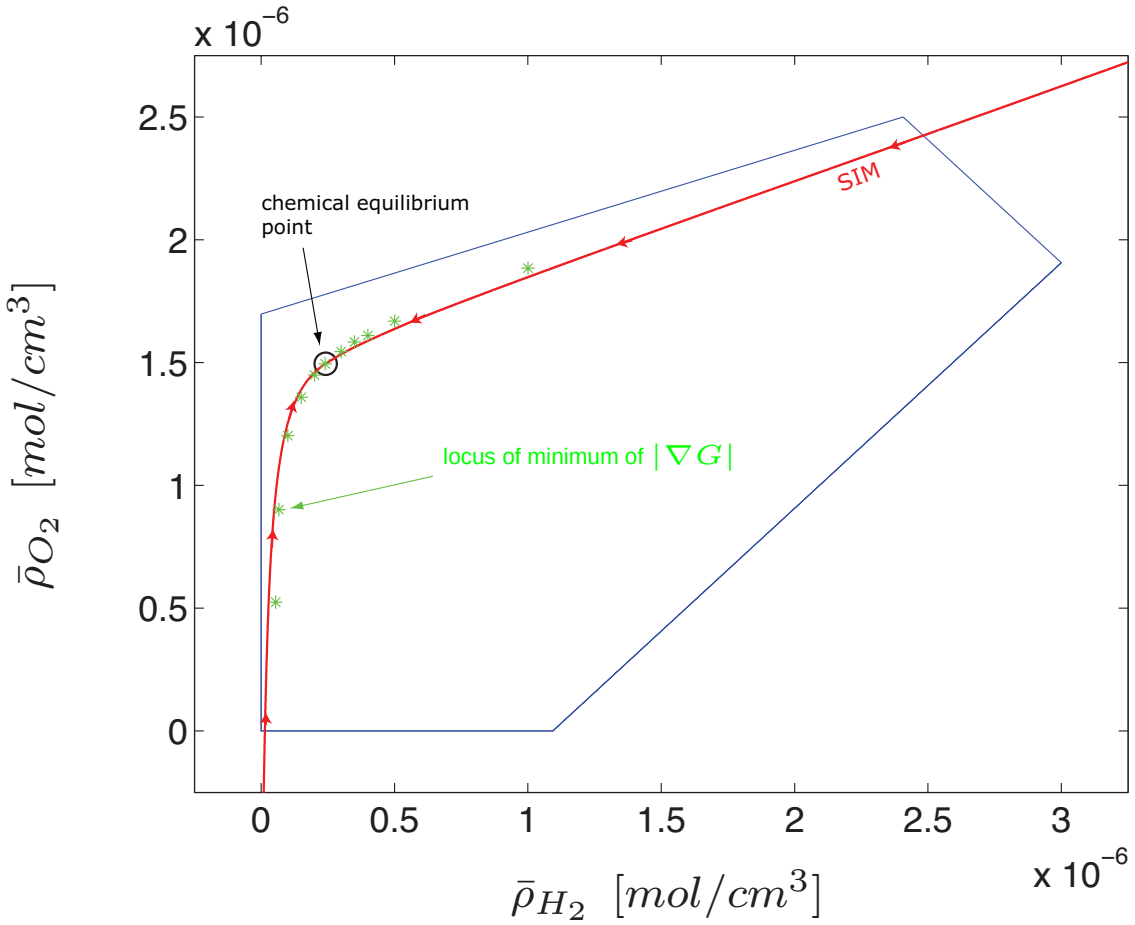
Detailed finite phase space

- Stiffness near equilibrium is $\mathcal{O}(10^2)$.



Relation with thermodynamics

- The local minimum of $|\nabla G|$ does not coincide with the SIM,



Summary

- Constructing the SIM is computationally efficient.
- Identifying all critical points, finite and infinite, play a major role in constructing the SIM.
- In constrast to the Poincaré sphere, it is easy to extend the projective geometry technique to higher dimensional systems, (*i.e.* $N = 9$).
- Away from chemical equilibrium, thermodynamic potentials do not correlate with the dynamics.

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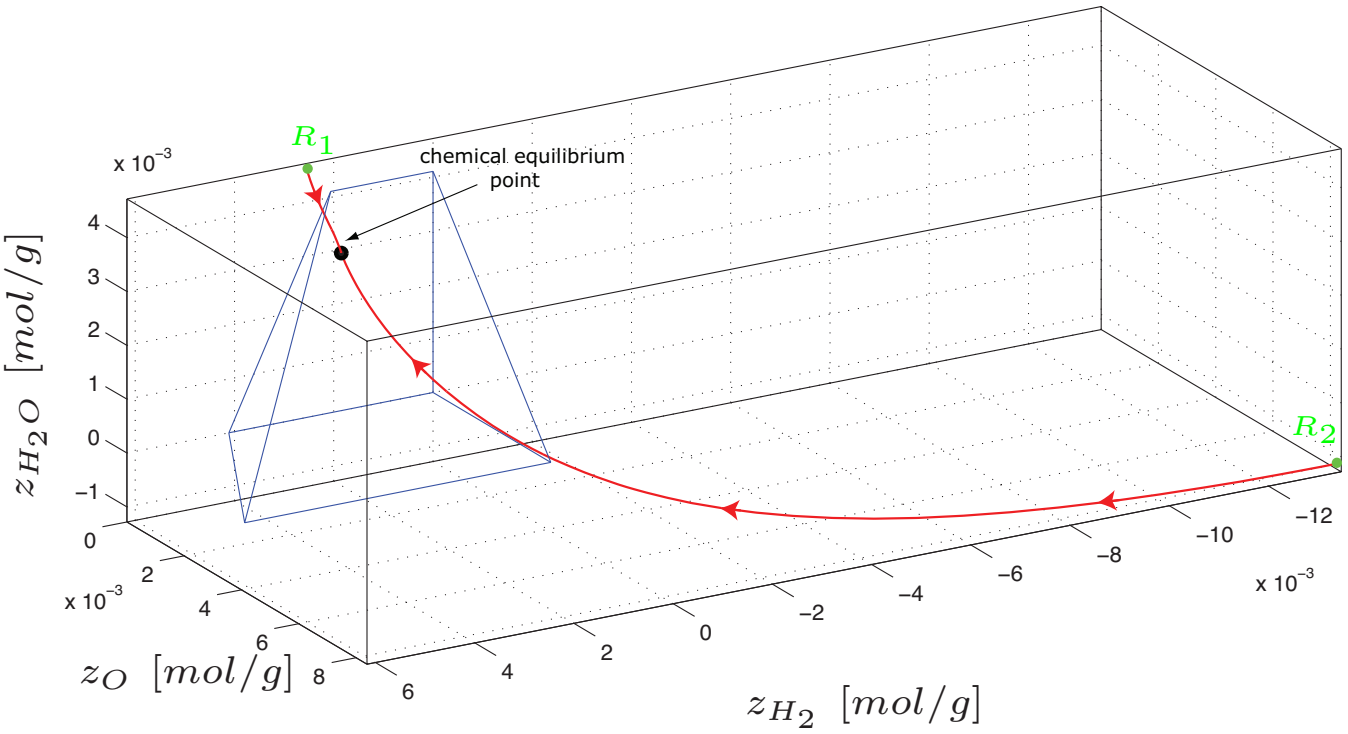
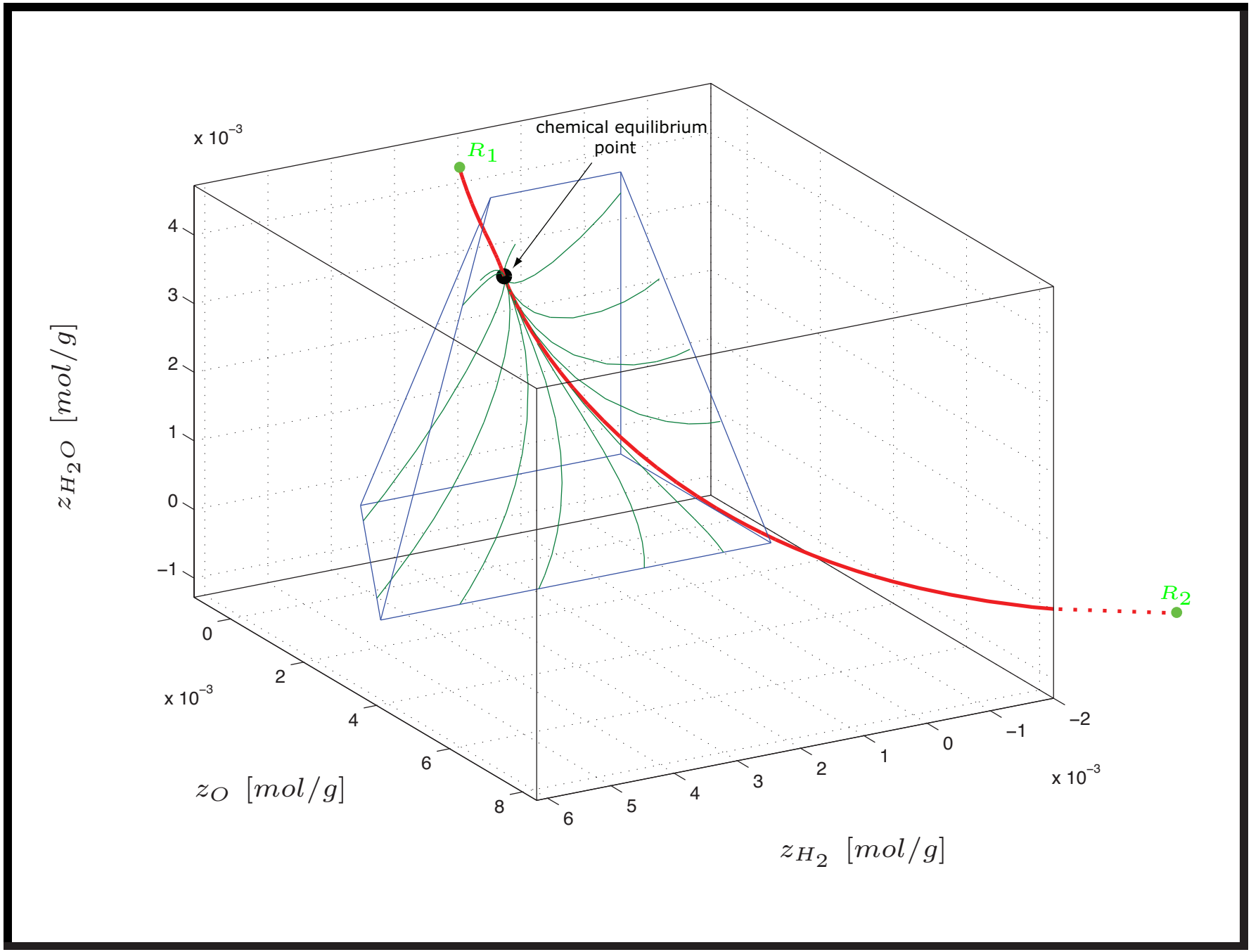
  - Center of Applied Mathematics, University of Notre Dame.

- The SIM for the system described in Ren *et al.*[a]



[a]Z. Ren, S. Pope, A. Vladimirsky, J. Guckenheimer, 2006, *J. Chem. Phys.*, **124** 114111.


chemical equilibrium point
R_1
R_2
x 10^{-3}
4
3
2
1
0
−1
z_{H_2O} $[mol/g]$
0
2
4
6
8
x 10^{-3}
z_O $[mol/g]$
6
5
4
3
2
1
0
−1
−2
x 10^{-3}
z_{H_2} $[mol/g]$