Probabilistic Lambert Problem: Connections with Optimal Mass Transport, Schrödinger Bridge and Reaction-Diffusion PDEs

Abhishek Halder

Department of Aerospace Engineering, Iowa State University
Department of Applied Mathematics, University of California Santa Cruz

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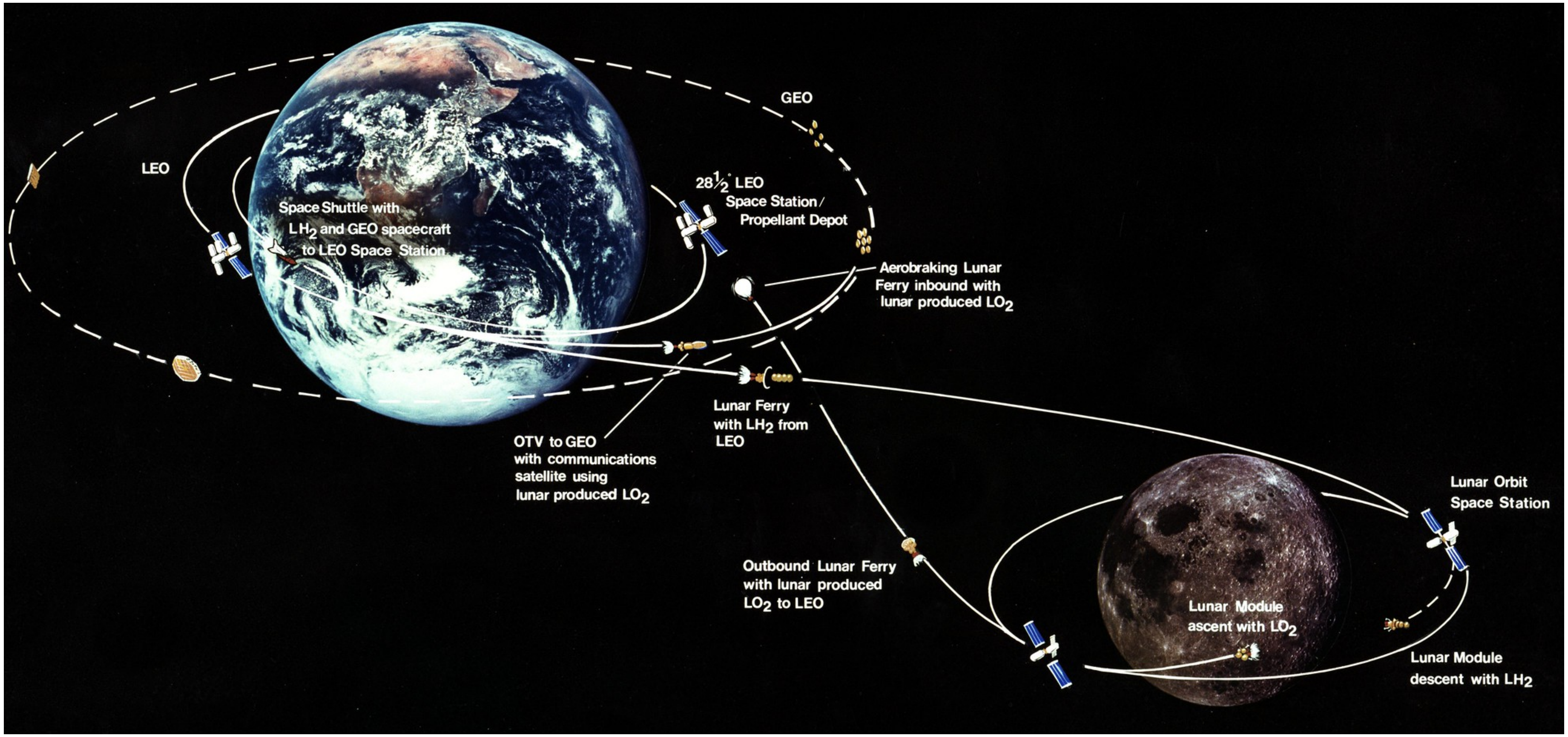
Probabilistic Lambert Problem: Connections with Optimal Mass Transport, Schrödinger Bridge, and Reaction-Diffusion PDEs*

Alexis M. H. Teter†, Iman Nodozi‡, and Abhishek Halder§

Probabilistic Lambert Problem

Lambert's Problem

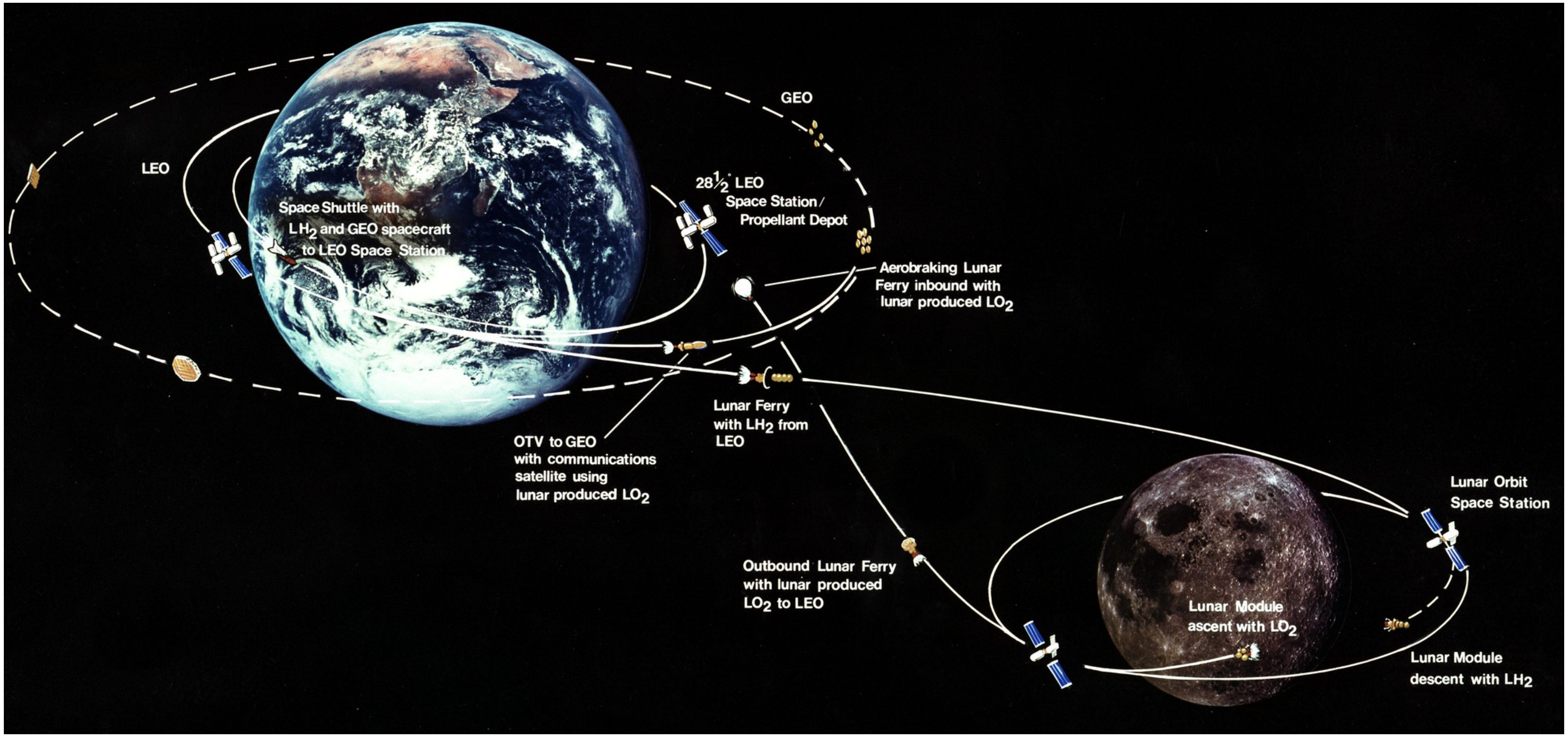


3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

Find velocity control policy $\dot{\boldsymbol{r}} := \boldsymbol{v}(t, \boldsymbol{r})$ such that

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boxed{\boldsymbol{r}(t = t_0) = \boldsymbol{r}_0(\text{ given }), \quad \boldsymbol{r}(t = t_1) = \boldsymbol{r}_1(\text{ given })}$$

Lambert's Problem



3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

ODE is 2nd order but endpoint boundary conditions are first order

Find velocity control policy $\dot{\boldsymbol{r}} := \boldsymbol{v}(t, \boldsymbol{r})$ such that

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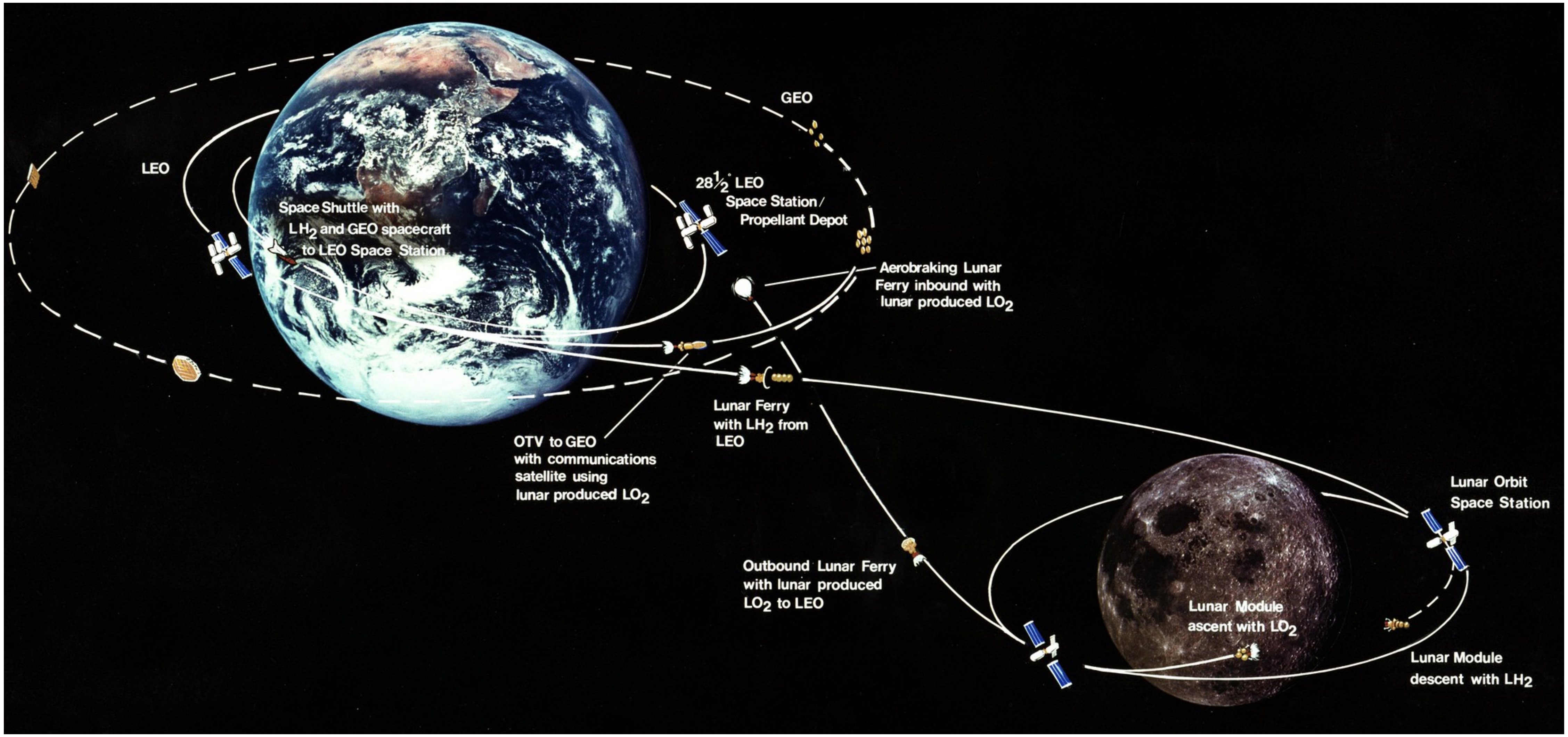
Lambert's Problem



3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

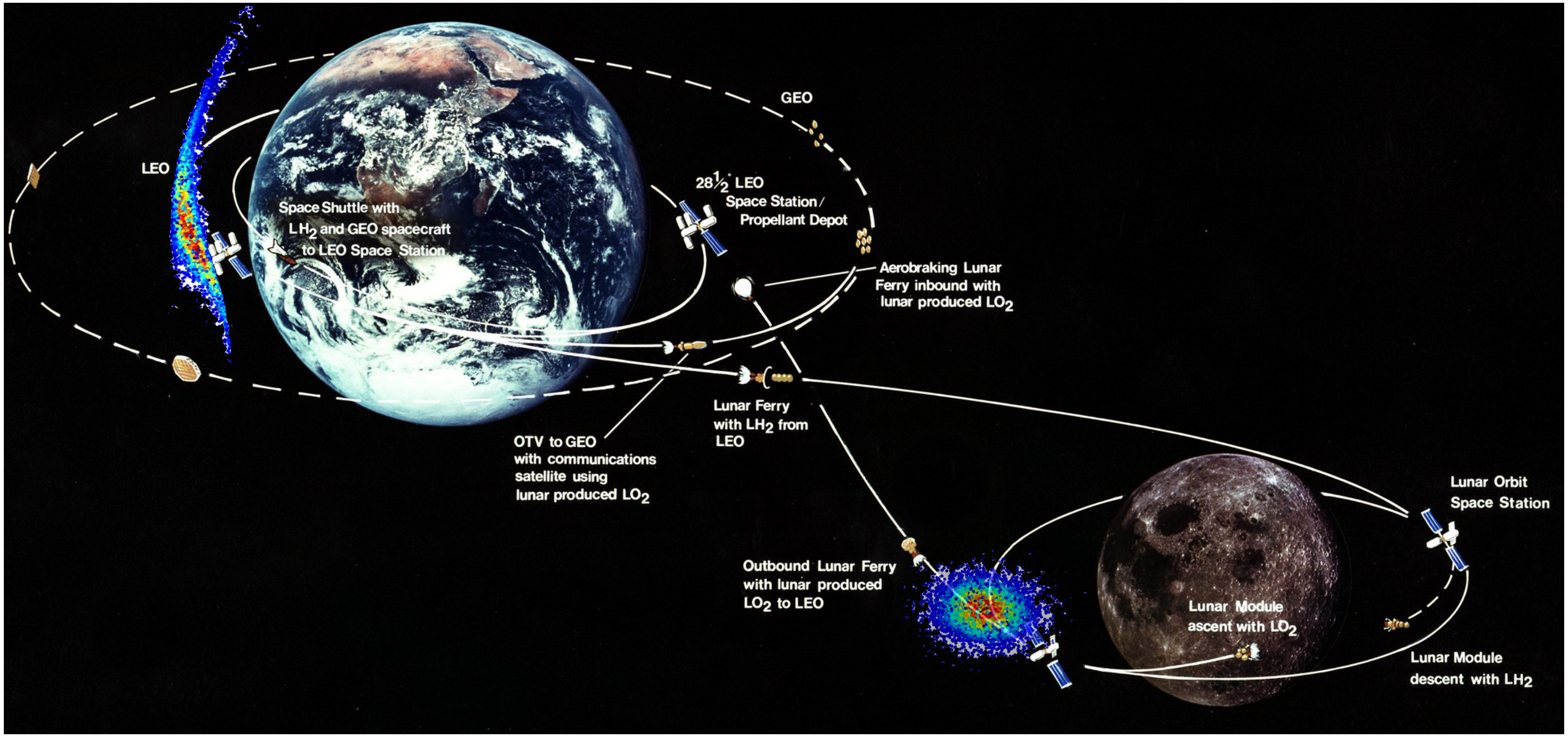
ODE is 2nd order but endpoint boundary conditions are first order

⇝ partially specified TPBVP

Find velocity control policy $\dot{\boldsymbol{r}} := \boldsymbol{v}(t, \boldsymbol{r})$ such that

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boxed{\boldsymbol{r}(t = t_0) = \boldsymbol{r}_0(\text{ given }), \quad \boldsymbol{r}(t = t_1) = \boldsymbol{r}_1(\text{ given })}$$

Probabilistic Lambert's Problem



3D position coordinate $\boldsymbol{r} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

Find velocity control policy $\dot{\boldsymbol{r}} := \boldsymbol{v}(t, \boldsymbol{r})$ such that

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boxed{\boldsymbol{r}(t = t_0) \sim \rho_0 \text{ (given)}, \quad \boldsymbol{r}(t = t_1) \sim \rho_1 \text{ (given)}}$$

The Beginning of Lambert's Problem

Named after polymath **Johann Heinrich Lambert (1728 - 1777)**

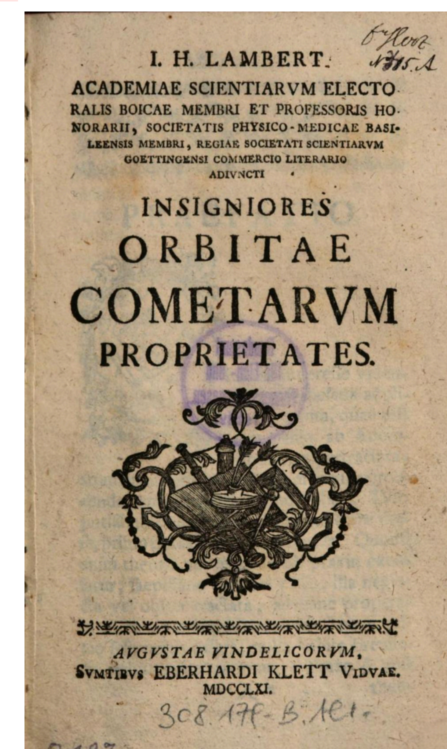
- known for first proof of irrationality of π, W function, area of a hyperbolic triangle

- special cases solved by Euler in 1743

- Lambert mentions this problem in letter to Euler in 1761

- solves the problem for parabolic, elliptic and hyperbolic Keplerian arcs in 1761 book

$$V(\boldsymbol{r}) = -\frac{\mu}{|\boldsymbol{r}|}$$



I. H. LAMBERT
ACADEMIAE SCIENTIARVM ELECTORALIS BOICAE MEMBRI ET PROFESSORIS HONORARII, SOCIETATIS PHYSICO-MEDICAE BASILEENSIS MEMBRI, REGIAE SOCIETATI SCIENTIARVM GOETTINGENSI COMMERCIO LITERARIO ADIVNCTI

INSIGNIORES ORBITAE COMETARVM PROPRIETATES.

AVGVSTAE VINDELICORVM,
SVMTIBVS EBERHARDI KLETT VIDVAE.
MDCCLXI.

- book receives high praise from Euler in 3 response letters

- alternative proofs by Lagrange (1780), Laplace (1798), Gauss (1809)

Modern History of Lambert's Problem

- Sustained interests for spacecraft guidance, missile interception

- 20th century astrodynamics research: fast computational algorithm, J2 effect in V

$$V(\boldsymbol{x}) = -\frac{\mu}{|\boldsymbol{x}|}\left(1 + \frac{J_2 R_{\text{Earth}}^2}{2|\boldsymbol{x}|^2}\left(1 - \frac{3z^2}{|\boldsymbol{x}|^2}\right)\right) \longrightarrow$$

Bounded and negative for $|\boldsymbol{x}|^2 \geq \mathrm{R}_{\text{Earth}}^2$

- 21st century interests in aerospace community: probabilistic Lambert's problem

- Endpoint uncertainties due to estimation errors, statistical performance

- State-of-the-art: approx. dynamics (linearization) + approx. statistics (covariance)

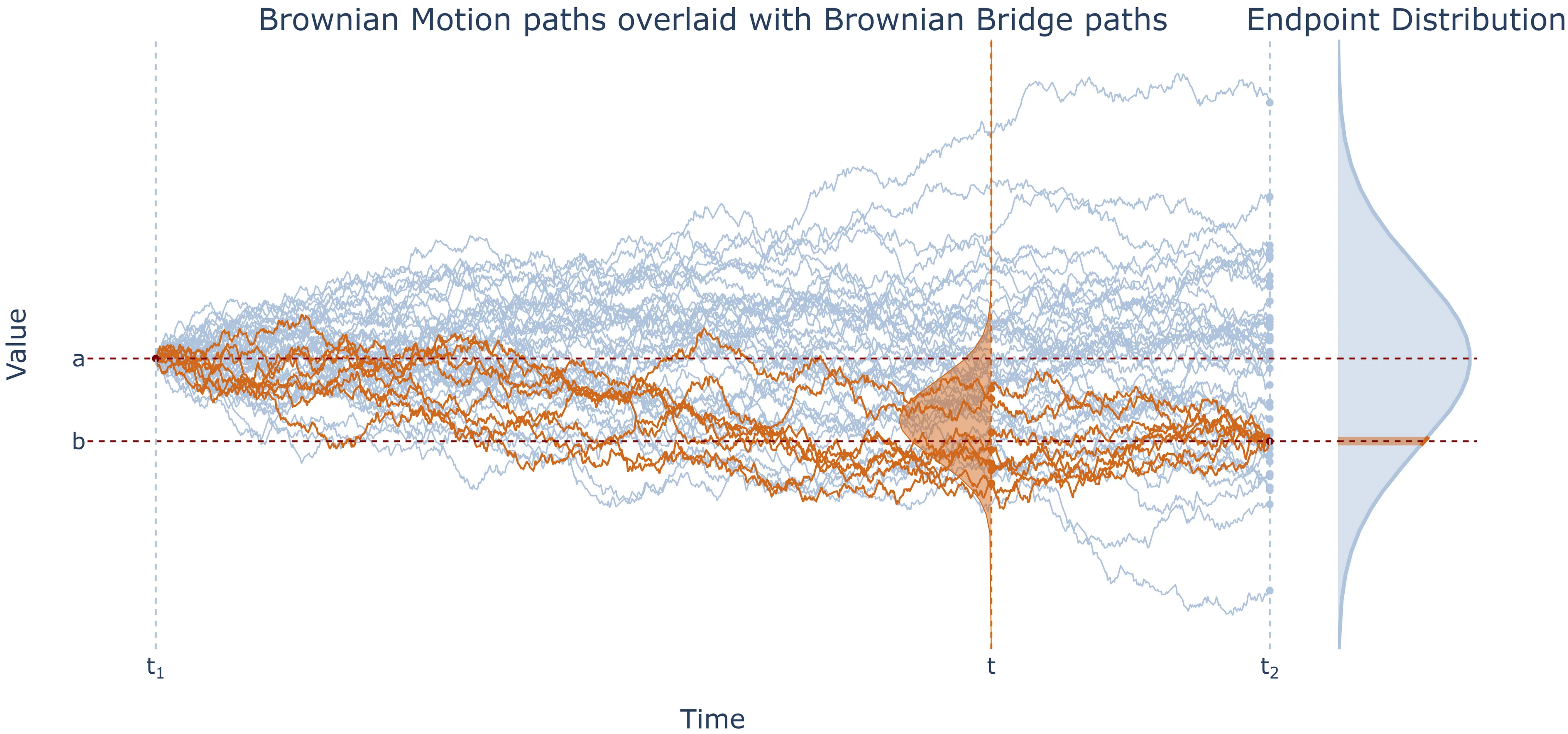
- Our contribution: connections with OMT and SBP

- Formulation/computation: non-parametric, well-posedness, optimality certificate

Schrödinger Bridge and Optimal Mass Transport

What is a Bridge

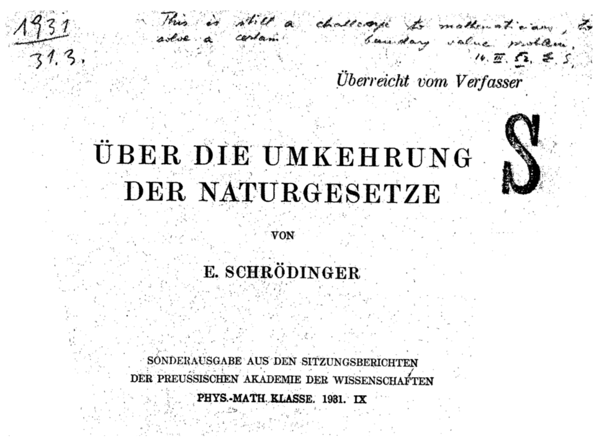
A stochastic process connecting two given states a, b in a given deadline $[t_1, t_2]$



Source: https://medium.com/@christopher.tabori/between-certainty-and-chance-tracing-the-probability-distribution-of-paths-of-brownian-bridges-b1f97eba638d

What is a Schrödinger Bridge

Prior physics = Brownian motion


1931
31.3.

This is still a challenge to mathematicians, to solve a certain boundary value problem.
14.IV.52. E.S.

Überreicht vom Verfasser

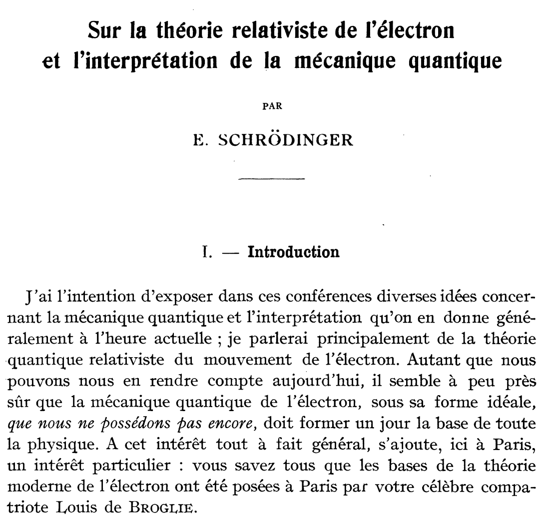
ÜBER DIE UMKEHRUNG DER NATURGESETZE

VON

E. SCHRÖDINGER

SONDERAUSGABE AUS DEN SITZUNGSBERICHTEN DER PREUSSISCHEN AKADEMIE DER WISSENSCHAFTEN PHYS.-MATH. KLASSE. 1931. IX

[1931]


Sur la théorie relativiste de l'électron et l'interprétation de la mécanique quantique

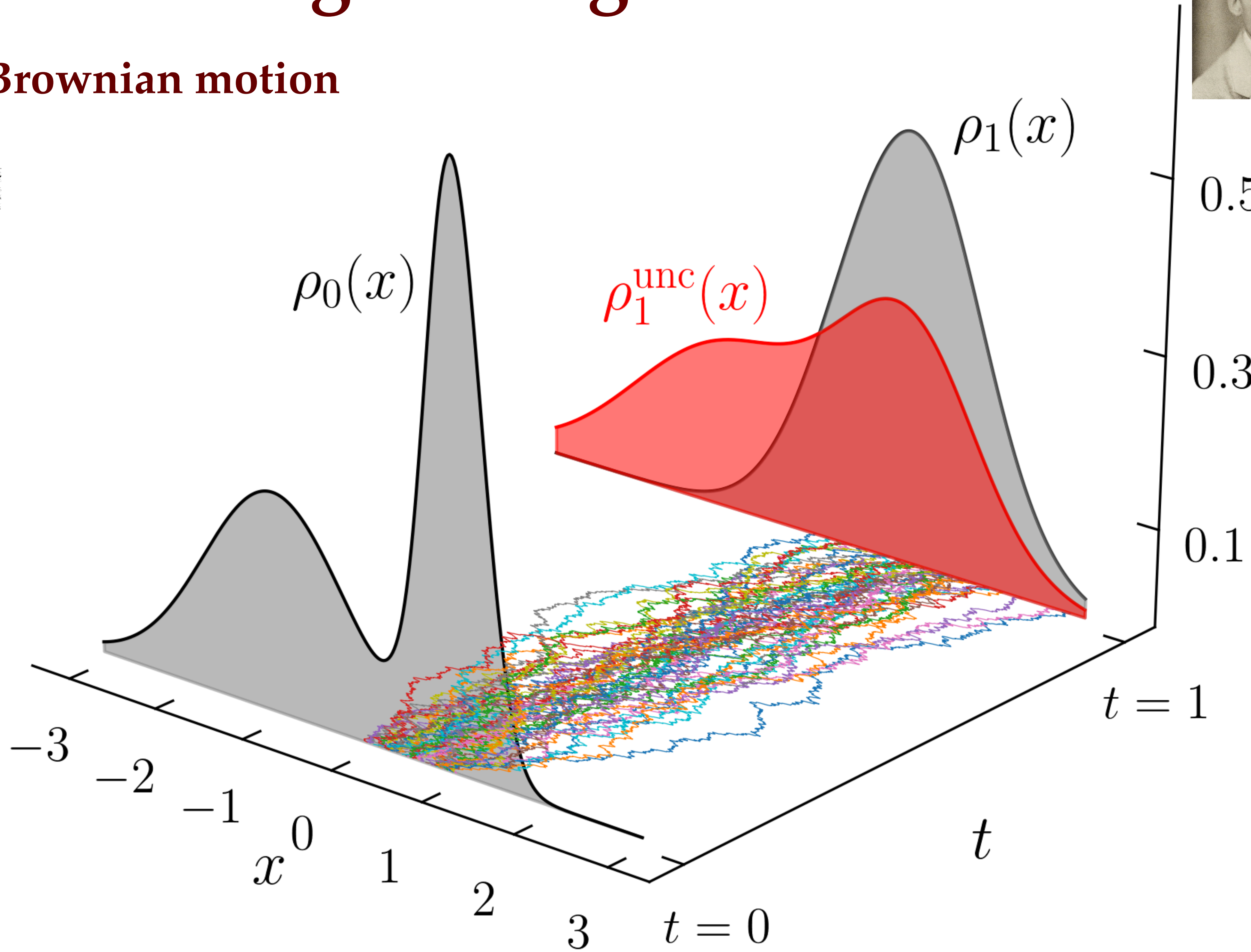
PAR

E. SCHRÖDINGER

I. — **Introduction**

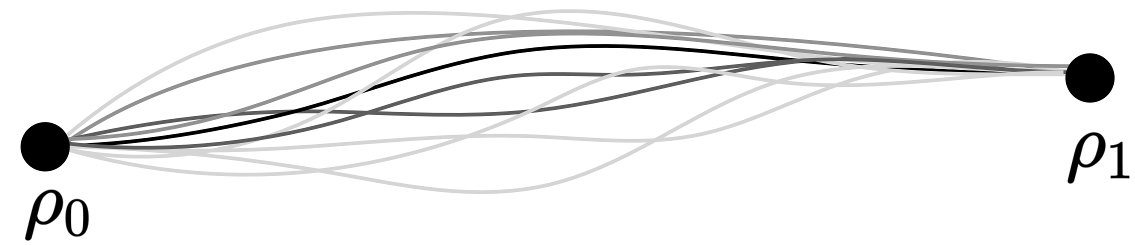
J'ai l'intention d'exposer dans ces conférences diverses idées concernant la mécanique quantique et l'interprétation qu'on en donne généralement à l'heure actuelle ; je parlerai principalement de la théorie quantique relativiste du mouvement de l'électron. Autant que nous pouvons nous en rendre compte aujourd'hui, il semble à peu près sûr que la mécanique quantique de l'électron, sous sa forme idéale, *que nous ne possédons pas encore*, doit former un jour la base de toute la physique. A cet intérêt tout à fait général, s'ajoute, ici à Paris, un intérêt particulier : vous savez tous que les bases de la théorie moderne de l'électron ont été posées à Paris par votre célèbre compatriote Louis de Broglie.

[1932]



Find the most likely explanation of observation vs prior physics mismatch

What is a Schrödinger Bridge



Path space $\Omega := C([t_0, t_1]; \mathbb{R}^n)$

Denote the collection of all probability measures on Ω as $\mathcal{M}(\Omega)$

$$\Pi_{01} := \{\mathbb{M} \in \mathcal{M}(\Omega) \mid \mathbb{M} \text{ has marginal } \rho_i \,\mathrm{d}\boldsymbol{x} \text{ at time } t_i \forall i \in \{0,1\}, \rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R}^n)\}$$

Schrödinger bridge = $\underset{\mathbb{P} \in \Pi_{01}}{\arg\inf} \quad D_{\mathrm{KL}}(\mathbb{P} \| \mathbb{W})$

Generated by Itô diffusion

Wiener measure

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{u}(t, \boldsymbol{x})\mathrm{d}t + \mathrm{d}\boldsymbol{w}(t)$$

Most parsimonious correction of prior physics

Constrained maximum likelihood problem on measure-valued paths

What is a Schrödinger bridge

Schrödinger bridge as large deviation principle: Sanov's theorem [1957]

$$\lim_{N\uparrow\infty} \log(\text{empiricial prob}_N \text{ under } \mathbb{W} \in \Pi_{01}) \asymp - \inf_{\mathbb{P}\in\Pi_{01}} D_{\mathrm{KL}}(\mathbb{P} \parallel \mathbb{W})$$

KL div as rate function

Schrödinger bridge as stochastic optimal control: [1990s]

$$\underset{\boldsymbol{u}\in\mathcal{U}}{\text{minimize}}\, \mathbb{E}\left[\int_{t_0}^{t_1} \frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^u)\|_2^2 \mathrm{d}t\right]$$

subject to

$$\mathrm{d}\boldsymbol{x}_t^u = \boldsymbol{u}(t,\boldsymbol{x}_t^u)\mathrm{d}t + \mathrm{d}\boldsymbol{w}_t$$

$$\boldsymbol{x}_t^u(t=t_0) \sim \rho_0, \quad \boldsymbol{x}_t^u(t=t_1) \sim \rho_1$$

What is a Schrödinger bridge

Schrödinger bridge as large deviation principle: Sanov's theorem [1957]

$$\lim_{N\uparrow\infty} \log(\text{empiricial prob}_N \text{ under } \mathbb{W} \in \Pi_{01}) \asymp -\inf_{\mathbb{P}\in\Pi_{01}} D_{\mathrm{KL}}(\mathbb{P} \parallel \mathbb{W})$$

KL divergence as rate function

Schrödinger bridge as stochastic optimal control: [1990s]

$$\underset{\boldsymbol{u}\in\mathcal{U}}{\text{minimize}}\, \mathbb{E}\left[\int_{t_0}^{t_1} \frac{1}{2}\|\boldsymbol{u}(t,\boldsymbol{x}_t^u)\|_2^2 \mathrm{d}t\right]$$

subject to

$$\mathrm{d}\boldsymbol{x}_t^u = \boldsymbol{u}(t,\boldsymbol{x}_t^u)\mathrm{d}t + \cancel{\mathrm{d}\boldsymbol{w}_t}$$

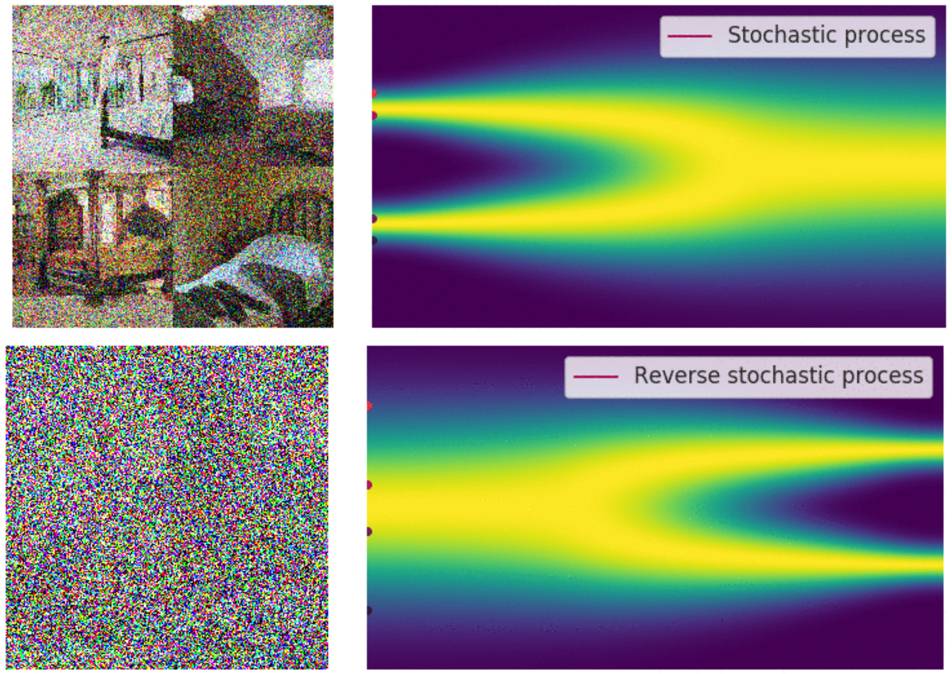
$$\boldsymbol{x}_t^u(t=t_0) \sim \rho_0, \quad \boldsymbol{x}_t^u(t=t_1) \sim \rho_1$$

0 Benamou-Brenier OMT [1999]

Resurgence of Schrödinger Bridge in AI

Diffusion models for generative AI

Source: https://yang-song.net/blog/2021/score/



NeurIPS 2021

Diffusion Schrödinger Bridge with Applications to Score-Based Generative Modeling

Valentin De Bortoli
Department of Statistics,
University of Oxford, UK

James Thornton
Department of Statistics,
University of Oxford, UK

Jeremy Heng
ESSEC Business School,
Singapore

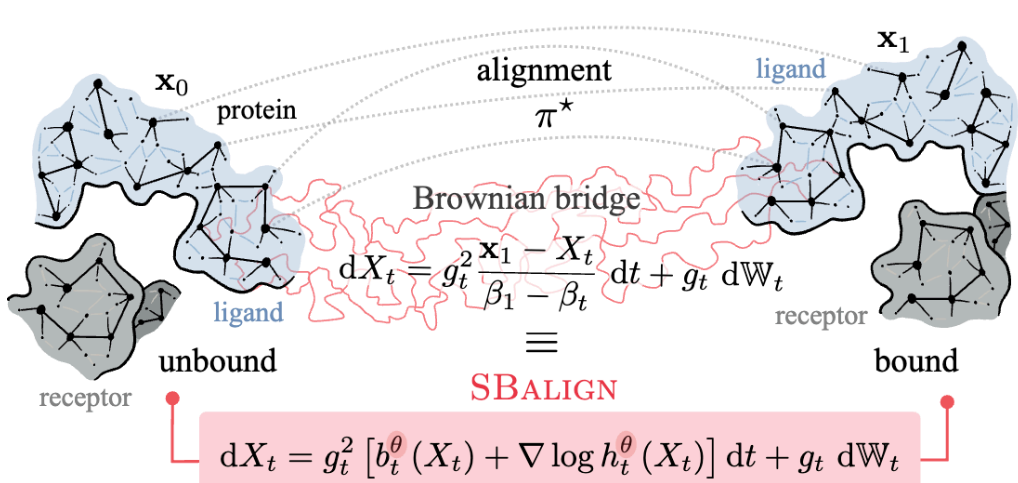
Arnaud Doucet
Department of Statistics,
University of Oxford, UK

UAI 2023

Aligned Diffusion Schrödinger Bridges

Vignesh Ram Somnath[*1,2] **Matteo Pariset**[*1,3] **Ya-Ping Hsieh**[1]
Maria Rodriguez Martinez[2] **Andreas Krause**[1] **Charlotte Bunne**[1]

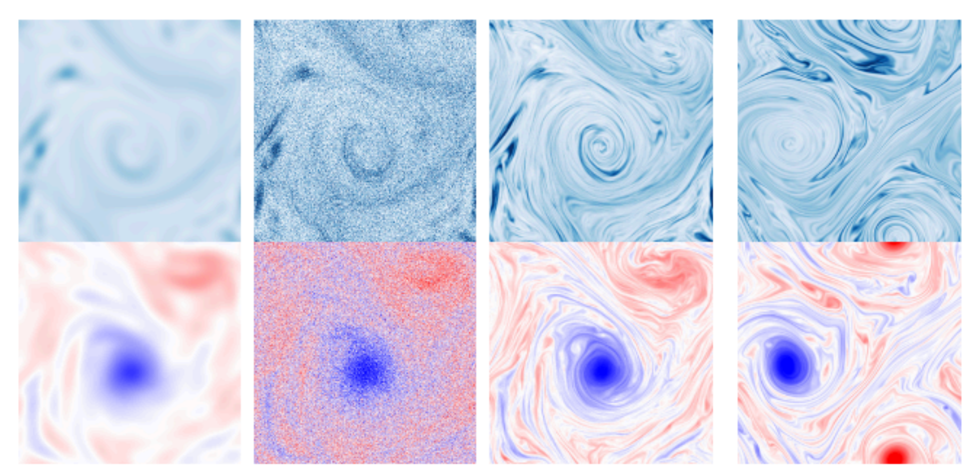
[1]Department of Computer Science, ETH Zürich
[2]IBM Research Zürich
[3]Department of Computer Science, EPFL



NeurIPS 2024

Diffusion Schrödinger Bridge Matching

Yuyang Shi[*] University of Oxford
Valentin De Bortoli[*] ENS ULM
Andrew Campbell University of Oxford
Arnaud Doucet University of Oxford



Low res **High res**

Back to Probabilistic Lambert Problem: Connecting Ideas

Connection with Optimal Control Problem (OCP)

Lambert Problem $\Leftrightarrow$ Deterministic OCP

Idea: use classical Hamiltonian mechanics to reformulate as deterministic OCP

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boldsymbol{r}(t=t_0) = \boldsymbol{r}_0(\text{ given }), \quad \boldsymbol{r}(t=t_1) = \boldsymbol{r}_1(\text{ given })$$

$$\Updownarrow$$

$$\underset{\boldsymbol{v}}{\arg\inf} \int_{t_0}^{t_1} \left(\frac{1}{2}\|\boldsymbol{v}\|_2^2 - V(\boldsymbol{r})\right) \mathrm{d}t$$

Gravitational potential pushed from dynamics to Lagrangian

$$\dot{\boldsymbol{r}} = \boldsymbol{v},$$

$$\boldsymbol{r}(t=t_0) = \boldsymbol{r}_0 \text{ (given)}, \quad \boldsymbol{r}(t=t_1) = \boldsymbol{r}_1 \text{ (given)}$$

Lambertian OMT (L-OMT)

Probabilistic Lambert Problem ⇔ Generalized OMT

$$\ddot{\boldsymbol{r}} = -\nabla_{\boldsymbol{r}} V(\boldsymbol{r}), \quad \boldsymbol{r}(t=t_0) \sim \rho_0 \text{ (given)}, \qquad \boldsymbol{r}(t=t_1) \sim \rho_1 \text{ (given)}$$

$$\Updownarrow$$

$$\underset{(\rho,\boldsymbol{v})}{\arg\inf} \quad \int_{t_0}^{t_1} \mathbb{E}_\rho \left[\frac{1}{2} \|\boldsymbol{v}\|_2^2 - \underbrace{V(\boldsymbol{r})}_{\text{Potential as state cost } (V=0 \text{ is OMT})} \right] \mathrm{d}t$$

$$\dot{\boldsymbol{r}} = \boldsymbol{v},$$

$$\boldsymbol{r}(t=t_0) \sim \rho_0 \text{ (given)}, \qquad \boldsymbol{r}(t=t_1) \sim \rho_1 \text{ (given)}$$

L-OMT as Density Steering

$$\underset{(\rho,\boldsymbol{v})}{\arg\inf} \int_{t_0}^{t_1} \mathbb{E}_\rho\left[\frac{1}{2}\|\boldsymbol{v}\|_2^2 - V(\boldsymbol{r})\right] \mathrm{d}t$$

$$\dot{\boldsymbol{r}} = \boldsymbol{v},$$

$$\boldsymbol{r}(t=t_0) \sim \rho_0 \text{ (given)}, \quad \boldsymbol{r}(t=t_1) \sim \rho_1 \text{ (given)}$$

$$\Updownarrow$$

$$\underset{(\rho,\boldsymbol{v})}{\arg\inf} \int_{t_0}^{t_1} \mathbb{E}_\rho\left[\frac{1}{2}\|\boldsymbol{v}\|_2^2 - V(\boldsymbol{r})\right] \mathrm{d}t$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}) = 0,$$

Liouville PDE

$$\rho(t=t_0,\cdot) = \rho_0, \quad \rho(t=t_1,\cdot) = \rho_1$$

Existence-Uniqueness of L-OMT Solution

Thm. (informal)
Existence-uniqueness guaranteed for V bounded C^1,
and ρ_0, ρ_1 with finite second moments

Proof idea.
Figalli's theory for OMT with Tonelli Lagrangians that are induced by action integrals

Connection to SBP with state cost

$$\underset{(\rho,\boldsymbol{v})\in\mathcal{P}_{01}\times\mathcal{V}}{\arg\inf} \int_{t_0}^{t_1}\int_{\mathbb{R}^n}\left(\frac{1}{2}|\boldsymbol{v}|^2 - V(\boldsymbol{x})\right)\rho(\boldsymbol{x},t)\,d\boldsymbol{x}dt$$

$$\frac{\partial\rho}{\partial t} + \nabla_{\boldsymbol{r}}\cdot(\rho\boldsymbol{v}) = 0,$$ — **Liouville PDE**

$$\rho(t=t_0,\cdot)=\rho_0, \quad \rho(t=t_1,\cdot)=\rho_1$$

Lambertian SBP (L-SBP)

$$\underset{(\rho,\boldsymbol{v})\in\mathcal{P}_{01}\times\mathcal{V}}{\arg\inf} \int_{t_0}^{t_1}\int_{\mathbb{R}^n}\left(\frac{1}{2}|\boldsymbol{v}|^2 - V(\boldsymbol{x})\right)\rho(\boldsymbol{x},t)\,d\boldsymbol{x}dt$$

Regularization > 0

$$\frac{\partial\rho}{\partial t} + \nabla_{\boldsymbol{r}}\cdot(\rho\boldsymbol{v}) = \varepsilon\Delta_{\boldsymbol{r}}\rho,$$ — **Fokker-Planck-Kolmogorov PDE**

$$\rho(t=t_0,\cdot)=\rho_0, \quad \rho(t=t_1,\cdot)=\rho_1$$

L-SBP Solution

Thm. (informal) Existence and uniqueness of L-SBP is guaranteed

$$V(\boldsymbol{x}) = -\frac{\mu}{|\boldsymbol{x}|}\left(1 + \frac{J_2 R_{\text{Earth}}^2}{2|\boldsymbol{x}|^2}\left(1 - \frac{3z^2}{|\boldsymbol{x}|^2}\right)\right) \longrightarrow$$

Bounded and negative for $|\boldsymbol{x}|^2 \geq \mathrm{R}_{\text{Earth}}^2$

Thm. (Necessary conditions of optimality for L-SBP)

Dual PDE

$$\frac{\partial \psi_\varepsilon}{\partial t} + \frac{1}{2}|\nabla_{\boldsymbol{x}}\psi_\varepsilon|^2 + \varepsilon\Delta_{\boldsymbol{x}}\psi_\varepsilon = -V(\boldsymbol{x})$$

Primal PDE

$$\frac{\partial \rho_\varepsilon^{\text{opt}}}{\partial t} + \nabla_{\boldsymbol{x}} \cdot \left(\rho_\varepsilon^{\text{opt}} \nabla_{\boldsymbol{x}}\psi_\varepsilon\right) = \varepsilon\Delta_{\boldsymbol{x}}\rho_\varepsilon^{\text{opt}}$$

$$\rho_\varepsilon^{\text{opt}}(t = t_0, \cdot) = \rho_0, \quad \rho_\varepsilon^{\text{opt}}(t = t_1, \cdot) = \rho_1$$

L-SBP Solution

Thm. (Hopf-Cole a.k.a. Fleming's log transform)

Change of variable $\left(\rho_{\varepsilon}^{\mathrm{opt}}, \psi\right) \mapsto (\widehat{\varphi}, \varphi)$ — **Schrödinger factors**

$$\widehat{\varphi}(t,\boldsymbol{r}) = \rho_{\varepsilon}^{\mathrm{opt}}(t,\boldsymbol{r}) \exp\left(-\frac{\psi(t,\boldsymbol{r})}{2\varepsilon}\right)$$

$$\varphi(t,\boldsymbol{r}) = \exp\left(\frac{\psi(t,\boldsymbol{r})}{2\varepsilon}\right)$$

results in a boundary-coupled system of forward-backward reaction-diffusion PDEs

$$\boxed{\begin{aligned} \frac{\partial \widehat{\varphi}}{\partial t} &= (\varepsilon \Delta_{\boldsymbol{r}} + V(\boldsymbol{r}))\widehat{\varphi} \longleftarrow \mathcal{L}_{\text{forward}}\widehat{\varphi} \\ \frac{\partial \varphi}{\partial t} &= -(\varepsilon \Delta_{\boldsymbol{r}} + V(\boldsymbol{r}))\varphi \longleftarrow \mathcal{L}_{\text{backward}}\varphi \\ \widehat{\varphi}(t=t_0,\cdot)\varphi(t=t_0,\cdot) &= \rho_0, \quad \widehat{\varphi}(t=t_1,\cdot)\varphi(t=t_1,\cdot) = \rho_1 \end{aligned}}$$

Optimally controlled joint state PDF: $\rho_{\varepsilon}^{\mathrm{opt}}(t,\boldsymbol{r}) = \widehat{\varphi}(t,\boldsymbol{r})\varphi(t,\boldsymbol{r})$

Optimal control: $\boldsymbol{v}_{\varepsilon}^{\mathrm{opt}}(t,\boldsymbol{r}) = 2\varepsilon \nabla_{\boldsymbol{r}} \log \varphi(t,\boldsymbol{r})$

L-SBP Computation via Schrödinger Factors

Recursion over pair $(\varphi_1, \hat{\varphi}_0)$

$$\begin{tikzcd}
\widehat{\varphi}_{\varepsilon,0}(\cdot) \arrow[r, "\int"] & \widehat{\varphi}_{\varepsilon}(\cdot, t = t_1) \arrow[d, "\rho_1(\cdot)/\widehat{\varphi}_{\varepsilon}(\cdot, t = t_1)"] \\
\varphi_{\varepsilon}(\cdot, t = t_0) \arrow[u, "\rho_0(\cdot)/\varphi_{\varepsilon}(\cdot, t = t_0)"] & \varphi_{\varepsilon,1}(\cdot) \arrow[l, "\int"]
\end{tikzcd}$$

$$\frac{\partial \widehat{\varphi}_{\varepsilon}}{\partial t} = \left(\varepsilon \Delta_{\boldsymbol{r}} + \frac{1}{2\varepsilon} V(\boldsymbol{r})\right) \widehat{\varphi}_{\varepsilon}$$

$$\frac{\partial \varphi_{\varepsilon}}{\partial t} = -\left(\varepsilon \Delta_{\boldsymbol{r}} + \frac{1}{2\varepsilon} V(\boldsymbol{r})\right) \varphi_{\varepsilon}$$

$$\rho_{\varepsilon}^{\text{opt}}(t = t_0, \cdot) = \rho_0, \quad \rho_{\varepsilon}^{\text{opt}}(t = t_1, \cdot) = \rho_1$$

Numerical Case Study

Prescribed time horizon $[t_0, t_1] \equiv [0,1]$ hours

Endpoint joint PDFs

$$\boldsymbol{x}_0 \sim \mathcal{N}(\mu_0, \Sigma_0)$$

$$\boldsymbol{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$$

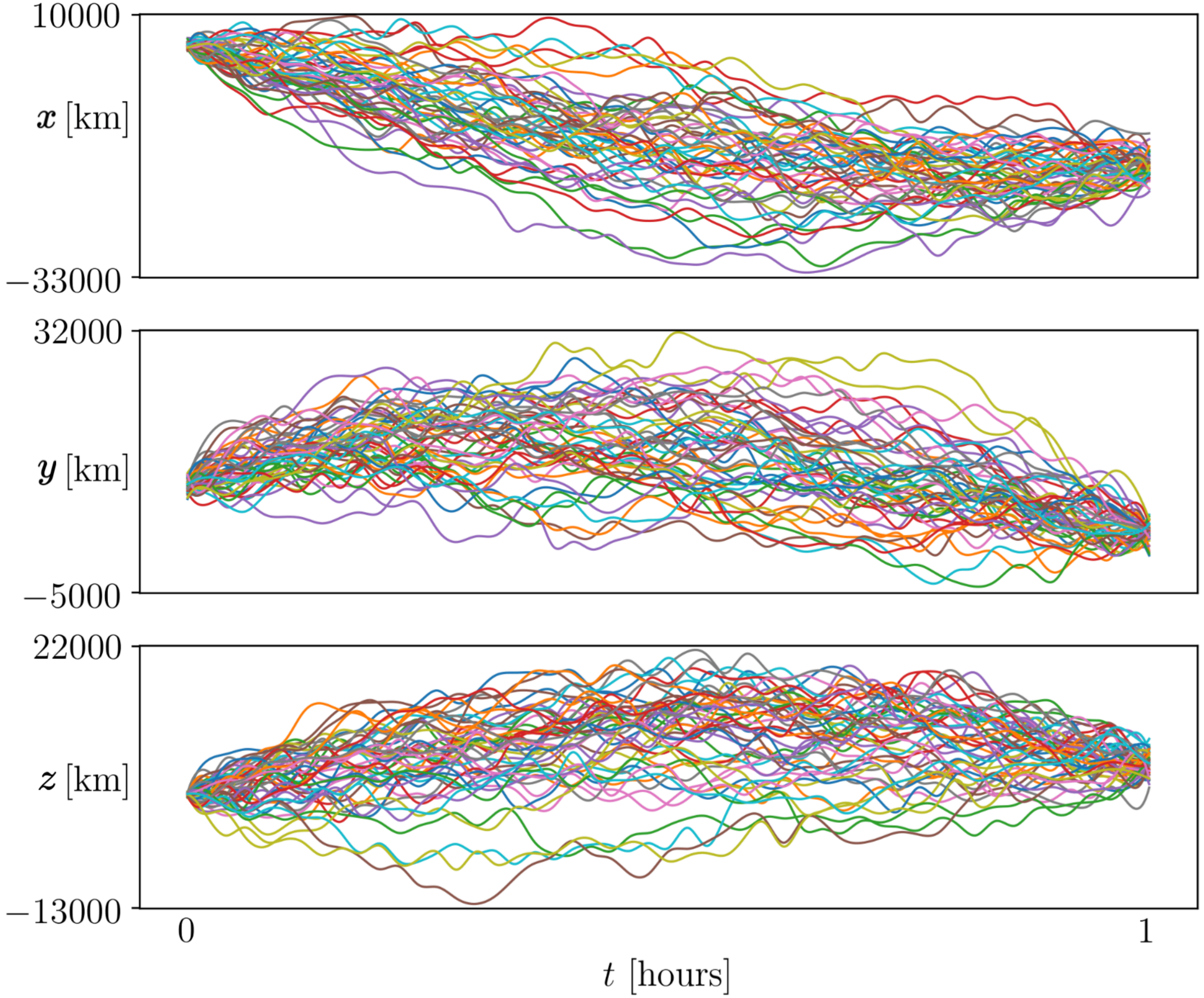
where

$$\mu_0 = \begin{pmatrix} 5000 \\ 10000 \\ 2100 \end{pmatrix}, \quad \mu_1 = \begin{pmatrix} -14600 \\ 2500 \\ 7000 \end{pmatrix}$$

$$\Sigma_0 = \frac{1}{100}\mathrm{diag}\left(\mu_0^2\right), \quad \Sigma_1 = \frac{1}{100}\mathrm{diag}\left(\mu_1^2\right),$$

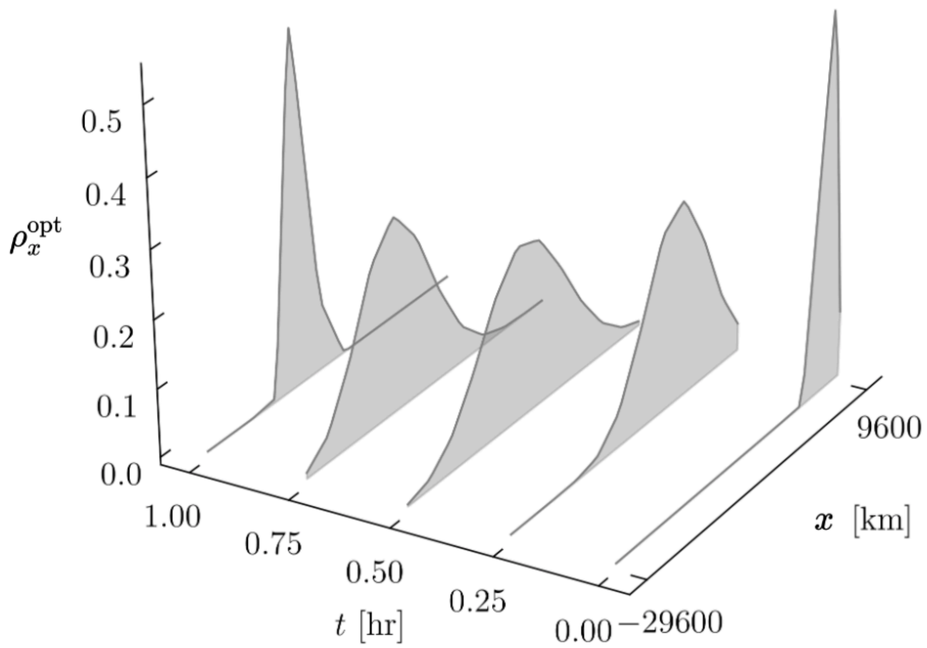
Numerical Case Study (cont.)

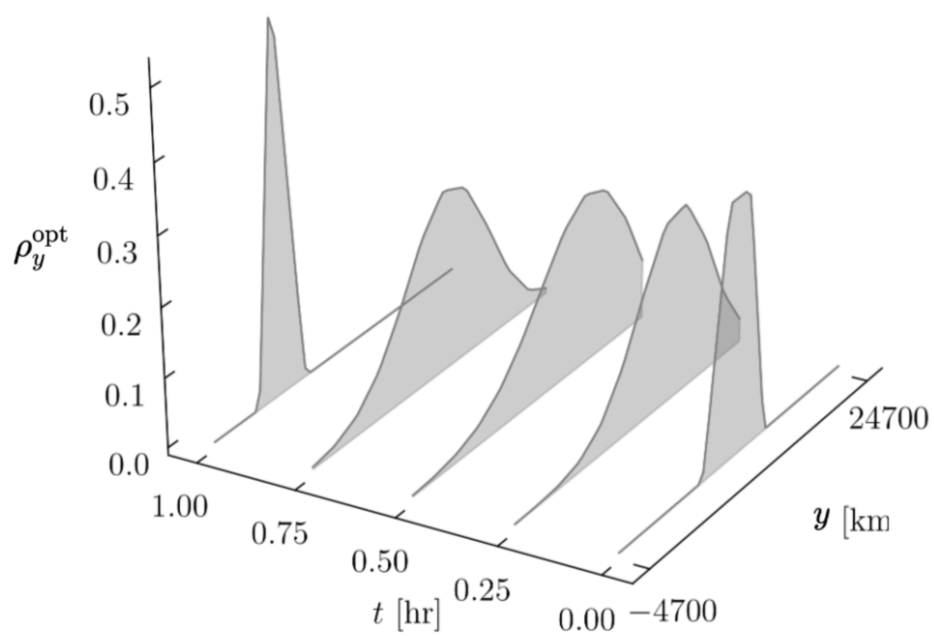
Optimally controlled closed loop state sample paths

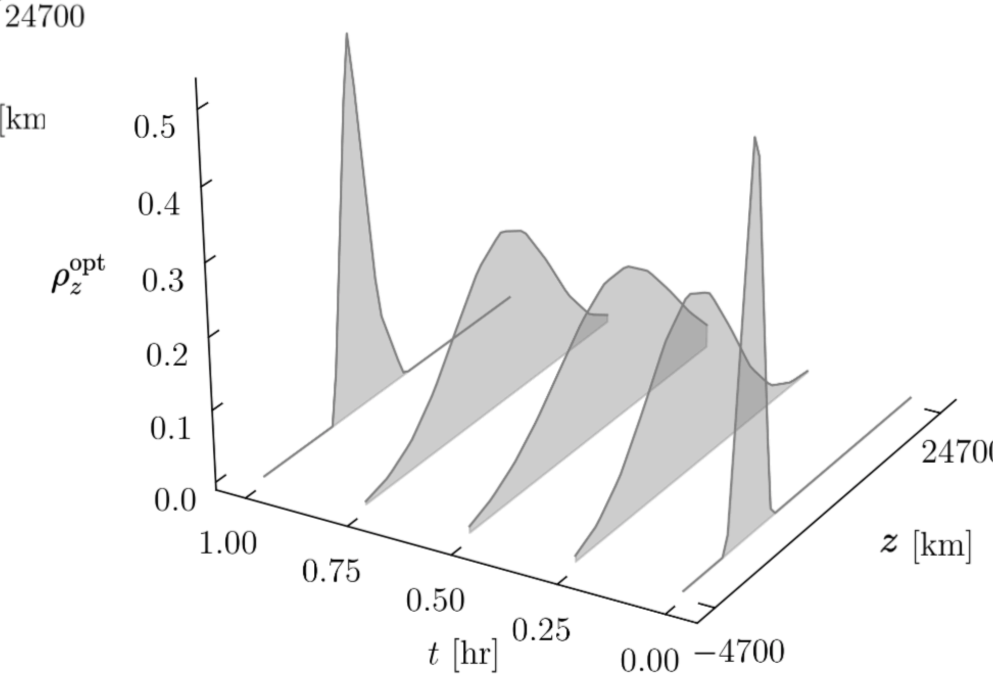


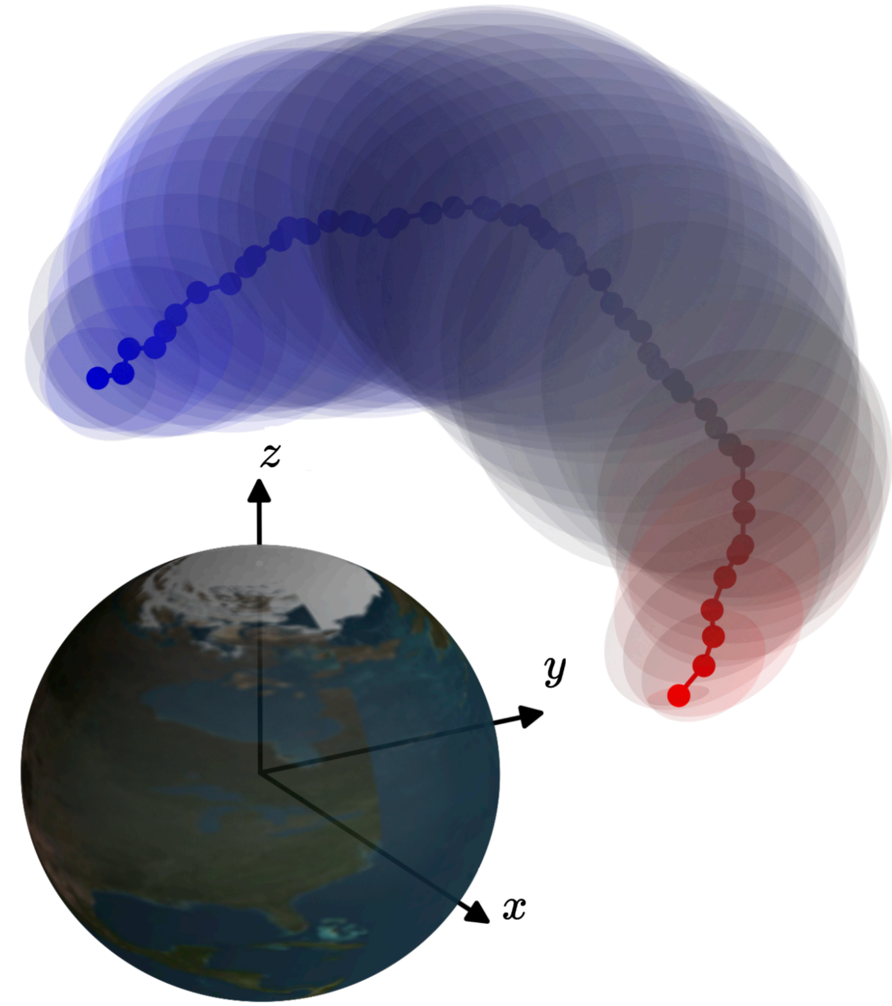
Numerical Case Study (cont.)

Univariate marginals for optimally controlled joint PDFs









Ongoing Efforts

- Find explicit Green's function for reaction-diffusion PDE with reaction rate equal to gravitational potential

- Connections with solution of time-dependent Schrödinger's equation in quantum mechanics for Hydrogen atom

Thank You

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