## PDMPs with ODE Dynamics

Sam Power<br>(joint with Sergio Bacallado)



November 15, 2018

## Overview

(1) PDMPs
(2) PDMPs for MCMC
(3) Construction of Algorithms
(4) Remarks, Open Questions, Takeaways

- Informally: Deterministic dynamics + Jump Process
- Informally: Deterministic dynamics + Jump Process
- Stochastic process $Z_{t}$ which
- Informally: Deterministic dynamics + Jump Process
- Stochastic process $Z_{t}$ which
(1) Follows a deterministic path, until
- Informally: Deterministic dynamics + Jump Process
- Stochastic process $Z_{t}$ which
(1) Follows a deterministic path, until

C己 An event occurs, at a certain rate, upon which

- Informally: Deterministic dynamics + Jump Process
- Stochastic process $Z_{t}$ which
(1) Follows a deterministic path, until
(2) An event occurs, at a certain rate, upon which
(3) The position jumps, and then
- Informally: Deterministic dynamics + Jump Process
- Stochastic process $Z_{t}$ which
(1) Follows a deterministic path, until
(2) An event occurs, at a certain rate, upon which
(3) The position jumps, and then
( Resumes following the deterministic path
- Informally: Deterministic dynamics + Jump Process
- Stochastic process $Z_{t}$ which
(1) Follows a deterministic path, until
(2) An event occurs, at a certain rate, upon which
(3) The position jumps, and then
- Resumes following the deterministic path



## Specifying a PDMP

- Today: PDMPs from ODEs


## Specifying a PDMP

- Today: PDMPs from ODEs
- Vector field $\phi(z)$
- Use dynamics $\frac{d z}{d t}=\phi(z)$


## Specifying a PDMP

- Today: PDMPs from ODEs
- Vector field $\phi(z)$
- Use dynamics $\frac{d z}{d t}=\phi(z)$
- Event rate $\lambda(z) \geqslant 0$
- Dictates how often events happen (inhomogeneous Poisson process)


## Specifying a PDMP

- Today: PDMPs from ODEs
- Vector field $\phi(z)$
- Use dynamics $\frac{d z}{d t}=\phi(z)$
- Event rate $\lambda(z) \geqslant 0$
- Dictates how often events happen (inhomogeneous Poisson process)
- Transition dynamics $Q\left(z \rightarrow d z^{\prime}\right)$
- Dictates what happens at events (Markov jump kernel)


## PDMPs for MCMC

- Want $\pi(d x)$, but work on extended target:


## PDMPs for MCMC

- Want $\pi(d x)$, but work on extended target:
- Set $z=(x, v)$.


## PDMPs for MCMC

- Want $\pi(d x)$, but work on extended target:
- Set $z=(x, v)$.
- Choose your own $\psi(d v)$.


## PDMPs for MCMC

- Want $\pi(d x)$, but work on extended target:
- Set $z=(x, v)$.
- Choose your own $\psi(d v)$.
- Target is then $\mu(d z)=\pi(d x) \psi(d v)$.


## PDMPs for MCMC

- Want $\pi(d x)$, but work on extended target:
- Set $z=(x, v)$.
- Choose your own $\psi(d v)$.
- Target is then $\mu(d z)=\pi(d x) \psi(d v)$.
- Typically, jumps fix $x \leadsto X_{t}$ has continuous sample paths.


## PDMPs for MCMC

- Want $\pi(d x)$, but work on extended target:
- Set $z=(x, v)$.
- Choose your own $\psi(d v)$.
- Target is then $\mu(d z)=\pi(d x) \psi(d v)$.
- Typically, jumps fix $x \leadsto X_{t}$ has continuous sample paths.
- Question:

> Given target measure $\mu$, vector field $\phi$, how can I build $(\lambda, Q)$ to sample $\mu$ ?

## Aside on Reversibility, Symmetry

- Reversibility
- Much MCMC work built on reversible methods
- PDMPs are generally non-reversible
- To design algorithms, locality is the important part


## Aside on Reversibility, Symmetry

- Reversibility
- Much MCMC work built on reversible methods
- PDMPs are generally non-reversible
- To design algorithms, locality is the important part
- Symmetry
- Existing PDMPs are highly symmetric (BPS, ZZ)
- A priori, not necessary to have symmetry
- Want to be able to use all ODEs!


## Time-Augmented PDMPs

- Idea:


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.
- Write $\phi(z, \tau)=\tau \cdot \phi(z)$; use dynamics $\frac{d z}{d t}=\phi(z, \tau)$


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.
- Write $\phi(z, \tau)=\tau \cdot \phi(z)$; use dynamics $\frac{d z}{d t}=\phi(z, \tau)$
- Solve system forwards and backwards in time


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.
- Write $\phi(z, \tau)=\tau \cdot \phi(z)$; use dynamics $\frac{d z}{d t}=\phi(z, \tau)$
- Solve system forwards and backwards in time
- Let $\lambda=\lambda(z, \tau)$


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.
- Write $\phi(z, \tau)=\tau \cdot \phi(z)$; use dynamics $\frac{d z}{d t}=\phi(z, \tau)$
- Solve system forwards and backwards in time
- Let $\lambda=\lambda(z, \tau)$
- Stipulate that, at events, $\tau \mapsto-\tau$, i.e.

$$
\begin{equation*}
Q\left((z, \tau) \rightarrow\left(d z^{\prime}, d \tau^{\prime}\right)\right)=Q^{\tau}\left(z \rightarrow d z^{\prime}\right) \cdot \delta\left(-\tau, d \tau^{\prime}\right) \tag{3}
\end{equation*}
$$

## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.
- Write $\phi(z, \tau)=\tau \cdot \phi(z)$; use dynamics $\frac{d z}{d t}=\phi(z, \tau)$
- Solve system forwards and backwards in time
- Let $\lambda=\lambda(z, \tau)$
- Stipulate that, at events, $\tau \mapsto-\tau$, i.e.

$$
\begin{equation*}
Q\left((z, \tau) \rightarrow\left(d z^{\prime}, d \tau^{\prime}\right)\right)=Q^{\tau}\left(z \rightarrow d z^{\prime}\right) \cdot \delta\left(-\tau, d \tau^{\prime}\right) \tag{3}
\end{equation*}
$$

- 'Trajectorial Reversibility' $\leadsto$ checking exactness becomes local!


## Time-Augmented PDMPs

- Idea:
(1) Introduce 'direction of time' variable $\tau \in\{ \pm 1\}$
(2) Target $\tilde{\mu}(d z, d \tau)=\mu(d z) R(d \tau)$.
- Write $\phi(z, \tau)=\tau \cdot \phi(z)$; use dynamics $\frac{d z}{d t}=\phi(z, \tau)$
- Solve system forwards and backwards in time
- Let $\lambda=\lambda(z, \tau)$
- Stipulate that, at events, $\tau \mapsto-\tau$, i.e.

$$
\begin{equation*}
Q\left((z, \tau) \rightarrow\left(d z^{\prime}, d \tau^{\prime}\right)\right)=Q^{\tau}\left(z \rightarrow d z^{\prime}\right) \cdot \delta\left(-\tau, d \tau^{\prime}\right) \tag{3}
\end{equation*}
$$

- 'Trajectorial Reversibility' $\leadsto$ checking exactness becomes local!
- 'in at $z$ forwards in time $=$ out at $z$ backwards in time'


## Choice of Event Rate (1)

- Consider 'probability current'

$$
\begin{equation*}
r(z, \tau) \triangleq \underbrace{\langle\nabla H(z), \phi(z, \tau)\rangle}_{\text {Energy Gain }}-\underbrace{\operatorname{div}_{z} \phi(z, \tau)}_{\text {Compressibility Penalty }} \tag{4}
\end{equation*}
$$

## Choice of Event Rate (1)

- Consider 'probability current'

$$
\begin{equation*}
r(z, \tau) \triangleq \underbrace{\langle\nabla H(z), \phi(z, \tau)\rangle}_{\text {Energy Gain }}-\underbrace{\operatorname{div}_{z} \phi(z, \tau)}_{\text {Compressibility Penalty }} \tag{4}
\end{equation*}
$$

- Define 'natural' event rate as

$$
\begin{equation*}
\lambda^{0}(z, \tau)=(r(z, \tau))_{+} \tag{5}
\end{equation*}
$$

where $(u)_{+}=\max (0, u)$

## Choice of Event Rate (1)

- Consider 'probability current'

$$
\begin{equation*}
r(z, \tau) \triangleq \underbrace{\langle\nabla H(z), \phi(z, \tau)\rangle}_{\text {Energy Gain }}-\underbrace{\operatorname{div}_{z} \phi(z, \tau)}_{\text {Compressibility Penalty }} \tag{4}
\end{equation*}
$$

- Define 'natural' event rate as

$$
\begin{equation*}
\lambda^{0}(z, \tau)=(r(z, \tau))_{+} \tag{5}
\end{equation*}
$$

where $(u)_{+}=\max (0, u)$

- Let $\gamma(z) \geqslant 0$ be some 'refreshment rate'.


## Choice of Event Rate (1)

- Consider 'probability current'

$$
\begin{equation*}
r(z, \tau) \triangleq \underbrace{\langle\nabla H(z), \phi(z, \tau)\rangle}_{\text {Energy Gain }}-\underbrace{\operatorname{div}_{z} \phi(z, \tau)}_{\text {Compressibility Penalty }} \tag{4}
\end{equation*}
$$

- Define 'natural' event rate as

$$
\begin{equation*}
\lambda^{0}(z, \tau)=(r(z, \tau))_{+} \tag{5}
\end{equation*}
$$

where $(u)_{+}=\max (0, u)$

- Let $\gamma(z) \geqslant 0$ be some 'refreshment rate'.
- We will take $\lambda(z, \tau)=\lambda^{0}(z, \tau)+\gamma(z)$


## Choice of Transition Dynamics

- Define 'jump measure':

$$
\begin{equation*}
J^{\tau}(d z) \propto \mu(d z) \lambda(z, \tau) \tag{6}
\end{equation*}
$$

## Choice of Transition Dynamics

- Define 'jump measure':

$$
\begin{equation*}
J^{\tau}(d z) \propto \mu(d z) \lambda(z, \tau) \tag{6}
\end{equation*}
$$

- Want trajectorial reversibility


## Choice of Transition Dynamics

- Define 'jump measure':

$$
\begin{equation*}
J^{\tau}(d z) \propto \mu(d z) \lambda(z, \tau) \tag{6}
\end{equation*}
$$

- Want trajectorial reversibility
- $\Longrightarrow$ Need jump chain reversible w.r.t. jump measure


## Choice of Transition Dynamics

- Define 'jump measure':

$$
\begin{equation*}
J^{\tau}(d z) \propto \mu(d z) \lambda(z, \tau) \tag{6}
\end{equation*}
$$

- Want trajectorial reversibility
- $\Longrightarrow$ Need jump chain reversible w.r.t. jump measure
- $\sim$ Choose $q^{\tau}\left(z \rightarrow d z^{\prime}\right)$ to be $J^{\tau}$-reversible


## Putting together the ingredients

## Theorem

If $(\phi, \lambda, Q)$ are chosen in this way, then the resulting PDMP is trajectorially reversible, and admits $\tilde{\mu}$ as a stationary measure.

## Putting together the ingredients

## Theorem

If $(\phi, \lambda, Q)$ are chosen in this way, then the resulting PDMP is trajectorially reversible, and admits $\tilde{\mu}$ as a stationary measure.

## Theorem

If $(\phi, \lambda, Q)$ is a trajectorially-reversible, $\tilde{\mu}$-stationary TA-PDMP, then $\exists \gamma \geqslant 0$ such that

$$
\begin{equation*}
\lambda(z, \tau)=\lambda^{0}(z, \tau)+\gamma(z) \tag{7}
\end{equation*}
$$

and for $\tau \in\{ \pm 1\}, Q^{\tau}$ is $J^{\tau}$-reversible

## Split PDMPs (1)

- Many PDMPs in use have different types of event


## Split PDMPs (1)

- Many PDMPs in use have different types of event
- Refreshment
- Zig-Zag
- Local BPS (Factor Graph)
- Subsampling


## Split PDMPs (1)

- Many PDMPs in use have different types of event
- Refreshment
- Zig-Zag
- Local BPS (Factor Graph)
- Subsampling
- ...
- Each event type affects different parts of the system


## Split PDMPs (1)

- Many PDMPs in use have different types of event
- Refreshment
- Zig-Zag
- Local BPS (Factor Graph)
- Subsampling
- ...
- Each event type affects different parts of the system
- Key point: Different event types correspond to decompositions of $r$


## Split PDMPs (2)

- $z=\left(z_{1}, \cdots, z_{D}\right), \tau=\left(\tau_{1}, \cdots, \tau_{D}\right) \in\{ \pm 1\}^{D}$
- $\phi(z, \tau)=\tau \odot \phi(z)=\left(\tau_{1} \phi_{1}(z), \cdots, \tau_{D} \phi_{D}(z)\right)$


## Split PDMPs (2)

- $z=\left(z_{1}, \cdots, z_{D}\right), \tau=\left(\tau_{1}, \cdots, \tau_{D}\right) \in\{ \pm 1\}^{D}$
- $\phi(z, \tau)=\tau \odot \phi(z)=\left(\tau_{1} \phi_{1}(z), \cdots, \tau_{D} \phi_{D}(z)\right)$
- Assume decomposition

$$
\begin{equation*}
r(z, \tau)=\sum_{j=1}^{M} r_{j}(z, \tau) \tag{8}
\end{equation*}
$$

and existence of involutions $\mathcal{F}_{j}:\{ \pm 1\}^{D} \rightarrow\{ \pm 1\}^{D}$ such that

$$
\begin{equation*}
r_{j}\left(z, \mathcal{F}_{j}(\tau)\right)=-r_{j}(z, \tau) \tag{9}
\end{equation*}
$$

## Split PDMPs (2)

- $z=\left(z_{1}, \cdots, z_{D}\right), \tau=\left(\tau_{1}, \cdots, \tau_{D}\right) \in\{ \pm 1\}^{D}$
- $\phi(z, \tau)=\tau \odot \phi(z)=\left(\tau_{1} \phi_{1}(z), \cdots, \tau_{D} \phi_{D}(z)\right)$
- Assume decomposition

$$
\begin{equation*}
r(z, \tau)=\sum_{j=1}^{M} r_{j}(z, \tau) \tag{8}
\end{equation*}
$$

and existence of involutions $\mathcal{F}_{j}:\{ \pm 1\}^{D} \rightarrow\{ \pm 1\}^{D}$ such that

$$
\begin{equation*}
r_{j}\left(z, \mathcal{F}_{j}(\tau)\right)=-r_{j}(z, \tau) \tag{9}
\end{equation*}
$$

- Events of type $j$ happen at rate $\lambda_{j}(z, \tau)$
- and then jump according to $Q_{j}^{\tau}\left(z \rightarrow d z^{\prime}\right) \cdot \delta\left(\mathcal{F}_{j}(\tau), d \tau^{\prime}\right)$


## Making Split-PDMPs work (1)

- Define

$$
\begin{align*}
& \lambda_{j}^{0}(z, \tau)=\left(r_{j}(z, \tau)\right)_{+}  \tag{10}\\
& \lambda_{j}(z, \tau)=\lambda_{j}^{0}(z, \tau)+\gamma_{j}(z, \tau) \tag{11}
\end{align*}
$$

## Making Split-PDMPs work (1)

- Define

$$
\begin{align*}
& \lambda_{j}^{0}(z, \tau)=\left(r_{j}(z, \tau)\right)_{+}  \tag{10}\\
& \lambda_{j}(z, \tau)=\lambda_{j}^{0}(z, \tau)+\gamma_{j}(z, \tau) \tag{11}
\end{align*}
$$

- Define

$$
\begin{equation*}
J_{j}^{\tau}(d z) \propto \mu(d z) \lambda_{j}(z, \tau) \tag{12}
\end{equation*}
$$

and for each $\tau \in\{ \pm 1\}^{D}$, take $Q_{j}^{\tau}$ to be $J_{j}^{\tau}$-reversible.

## Making Split-PDMPs work (1)

- Define

$$
\begin{align*}
& \lambda_{j}^{0}(z, \tau)=\left(r_{j}(z, \tau)\right)_{+}  \tag{10}\\
& \lambda_{j}(z, \tau)=\lambda_{j}^{0}(z, \tau)+\gamma_{j}(z, \tau) \tag{11}
\end{align*}
$$

- Define

$$
\begin{equation*}
J_{j}^{\tau}(d z) \propto \mu(d z) \lambda_{j}(z, \tau) \tag{12}
\end{equation*}
$$

and for each $\tau \in\{ \pm 1\}^{D}$, take $Q_{j}^{\tau}$ to be $J_{j}^{\tau}$-reversible.

## Theorem

This leads to trajectorially-reversible, $\tilde{\mu}$-stationary Split PDMPs.

## Making Split-PDMPs work (1)

- Define

$$
\begin{align*}
& \lambda_{j}^{0}(z, \tau)=\left(r_{j}(z, \tau)\right)_{+}  \tag{10}\\
& \lambda_{j}(z, \tau)=\lambda_{j}^{0}(z, \tau)+\gamma_{j}(z, \tau) \tag{11}
\end{align*}
$$

- Define

$$
\begin{equation*}
J_{j}^{\tau}(d z) \propto \mu(d z) \lambda_{j}(z, \tau) \tag{12}
\end{equation*}
$$

and for each $\tau \in\{ \pm 1\}^{D}$, take $Q_{j}^{\tau}$ to be $J_{j}^{\tau}$-reversible.

## Theorem

This leads to trajectorially-reversible, $\tilde{\mu}$-stationary Split PDMPs.

## Theorem

Given a fixed splitting, all trajectorially-reversible, $\tilde{\mu}$-stationary Split PDMPs take this form.

## Algorithm Design Pipeline (1)

- Non-negotiable: we want samples from $\pi(d x)$.


## Algorithm Design Pipeline (1)

- Non-negotiable: we want samples from $\pi(d x)$.
(1) Decide on $v$.
(2) Decide on $\phi$.
© Decide on $\psi(d v)$ (and hence $\mu$ ).


## Algorithm Design Pipeline (1)

- Non-negotiable: we want samples from $\pi(d x)$.
(1) Decide on $v$.
(2) Decide on $\phi$.
(3) Decide on $\psi(d v)$ (and hence $\mu$ ).
(-) Write down $r$, decide on a splitting.


## Algorithm Design Pipeline (1)

- Non-negotiable: we want samples from $\pi(d x)$.
(1) Decide on $v$.
(3) Decide on $\phi$.
(3) Decide on $\psi(d v)$ (and hence $\mu$ ).
(-) Write down $r$, decide on a splitting.
(0) Write down $\lambda^{0}$, decide on $\gamma$ (and hence $\lambda$ ).


## Algorithm Design Pipeline (1)

- Non-negotiable: we want samples from $\pi(d x)$.
(1) Decide on $v$.
(2) Decide on $\phi$.
(3) Decide on $\psi(d v)$ (and hence $\mu$ ).
(-) Write down $r$, decide on a splitting.
(0) Write down $\lambda^{0}$, decide on $\gamma$ (and hence $\lambda$ ).
( Decide on $Q$.


## Algorithm Design Pipeline (2)

- Choosing $Q$ is often least obvious; order of preference:


## Algorithm Design Pipeline (2)

- Choosing $Q$ is often least obvious; order of preference:
(1) Sample from $J^{\tau}$ directly.


## Algorithm Design Pipeline (2)

- Choosing $Q$ is often least obvious; order of preference:
(1) Sample from $J^{\tau}$ directly.
(2) Sample from its restriction to a finite set. (e.g. BPS)


## Algorithm Design Pipeline (2)

- Choosing $Q$ is often least obvious; order of preference:
(1) Sample from $J^{\tau}$ directly.
(2) Sample from its restriction to a finite set. (e.g. BPS)
© (Use a Metropolis-Hastings step).


## Algorithm Design Pipeline (2)

- Choosing $Q$ is often least obvious; order of preference:
(1) Sample from $J^{\tau}$ directly.
(2) Sample from its restriction to a finite set. (e.g. BPS)
© (Use a Metropolis-Hastings step).
- Choosing $\psi$ could make a big difference; dictates $\mu$.
- Can have $\psi(d v \mid x)$ (relatively unexplored)


## Algorithm Design Pipeline (2)

- Choosing $Q$ is often least obvious; order of preference:
(1) Sample from $J^{\tau}$ directly.
(2) Sample from its restriction to a finite set. (e.g. BPS)
(3) (Use a Metropolis-Hastings step).
- Choosing $\psi$ could make a big difference; dictates $\mu$.
- Can have $\psi(d v \mid x)$ (relatively unexplored)
- Choosing $\phi$ : some room for creativity here.


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs
- Conjecture: Split as little as possible


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs
- Conjecture: Split as little as possible
- Conjecture: Refresh as little as possible


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs
- Conjecture: Split as little as possible
- Conjecture: Refresh as little as possible
- Pinch of salt / 'Pre-Asymptopia': Maire, Vialaret (2018)


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs
- Conjecture: Split as little as possible
- Conjecture: Refresh as little as possible
- Pinch of salt / 'Pre-Asymptopia': Maire, Vialaret (2018)
- Implementation remains challenging
- Splittings may help


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs
- Conjecture: Split as little as possible
- Conjecture: Refresh as little as possible
- Pinch of salt / 'Pre-Asymptopia': Maire, Vialaret (2018)
- Implementation remains challenging
- Splittings may help
- Speculation: Better dynamics $\phi \sim$ opportunities


## Remarks, Open Questions, Takeaways

- Andrieu, Livingstone (2018): Peskun-type ordering for (some) PDMPs
- Conjecture: Split as little as possible
- Conjecture: Refresh as little as possible
- Pinch of salt / 'Pre-Asymptopia': Maire, Vialaret (2018)
- Implementation remains challenging
- Splittings may help
- Speculation: Better dynamics $\phi \sim$ opportunities
- Curiosity: Tempering?


## Thank you!

