From particle methods to hybrid semi-lagrangian schemes

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Outline

1. Low-noise particle methods (with polynomial shape transformations)

2. A forward-backward lagrangian (FBL) method
Motivation: improvement of existing particle codes
Classical approaches to particle denoising

- represent $f$ with smooth particle shapes $\varphi_{\varepsilon}$

$$f_{h,\varepsilon}^n(x) = \sum_{k \in \mathbb{Z}^d} w_k \varphi_{\varepsilon}(x-x_k^n), \quad \begin{cases} x_k^n & : \text{particle center, pushed along fwd flow } F^n \\ \varepsilon & : \text{particle size, } h_k \sim x_k^0 \end{cases}$$

- take $\varepsilon \gg h$ according to the classical estimate (Beale & Majda, Raviart, 80’s)

$$\|f_{h,\varepsilon}^n - f^n\|_{L^\infty} \leq \sup_x \left| \langle f_{h}^n - f^n, \psi_x, \varepsilon \rangle \right| + \|f^n * \varphi_{\varepsilon} - f^n\|_{L^\infty} \lesssim \left( \frac{h}{\varepsilon} \right)^2 + \varepsilon^2$$

  - requires huge numbers of particles
  - extended particle overlapping

- or take $\varepsilon \sim h$ and use periodic remappings

  - oscillations are smoothed out, but numerical diffusion introduced
  - accurate approximations exist (adaptive, high order, ...) but not fully satisfactory

Hybrid method: particles with remappings (Denavit, FSL)
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The linearly-transformed particle (LTP) method

- Each particle has a weight $w^n_k$, a center $x^n_k$ and a deformation matrix $D^n_k$

$$f^n_h(x) = \sum_{k \in \mathbb{Z}^d} w^n_k \varphi_h(D^n_k(x - x^n_k)) \quad (\varepsilon = h)$$

- LTP = exact transport of $\varphi_h(\cdot - x^n_0)$ along $\tilde{F}^n_{h,k} : x \rightarrow x^n_k + J^n_k(x - x^n_k)$
  - $J^n_k$ : fwd Jacobian approximated by FD, using current position of particles
  - straightforward inversion : $(\tilde{F}^n_{h,k})^{-1} : x \rightarrow x^n_0 + (J^n_k)^{-1}(x - x^n_k)$
  - remappings still needed to avoid unlimited stretching

- Math : (Hou, 1990), (Cohen and Perthame, 2000), Plasma physics : (Bateson and Hewett, 1998), (Hewett, 2003), (Alard and Colombi 2005)...

Supp($\varphi^0_{h,k}$) = $x^n_k + h[-c, c]^2$

Supp($\varphi^n_{h,k}$) = $x^n_k + (D^n_k)^{-1}(h[-c, c]^2)$
The quadratically-transformed particle method (QTP)

- Each QTP has the attributes of an LTP + additional matrices \((Q^n_k)_i, i = 0, 1\)

\[
f^n_h(x) \approx \sum_{k \in \mathbb{Z}^d} w^n_k \varphi_h \left( D^n_k(x - x^n_k) + \frac{1}{2} \sum_{j_1, j_2} ((Q^n_k)_{i, j_1, j_2}(x - x^n_k)_{j_1}(x - x^n_k)_{j_2})_{i=0,1} \right)
\]

- QTP transport = push of the center + quadratic deformation of the shape
  - Hessian matrices of the flow computed using current position of particles
  - remappings still needed to avoid unlimited stretching
  - care needed: defining the particle support is not straightforward

- New method (see MCP ’15)
Summing up: polynomial transport of particle shapes

- **principle**: transport the particle \( \varphi_{h,k}^0(x) := \varphi_h(x - x_k^0) \) with

\[
\tilde{T}_h^{n,(r)} \varphi_{h,k}^0(x) := \varphi_h(\tilde{B}_{h,k}^{n,(r)}(x) - x_k^0), \quad \tilde{B}_{h,k}^{n,(r)} \approx \tilde{B}^n
\]

- **order** \( r = 0 \) (PIC / FSL): use

\[
\tilde{B}_{h,k}^{n,(0)}(x) := x_k^0 + (x - x_k^n) \quad \text{with} \quad x_k^n := \tilde{F}^n(x_k^0)
\]

- **order** \( r = 1 \) (LTP): use

\[
\tilde{B}_{h,k}^{n,(1)}(x) := x_k^0 + D_k^n(x - x_k^n) \quad \text{with} \quad (D_k^n)_{i,j} := \partial_{j}(\tilde{B}^n)_{i}(x_k^n)
\]

- **order** \( r = 2 \) (QTP): use

\[
\tilde{B}_{h,k}^{n,(2)}(x) := x_k^0 + D_k^n(x - x_k^n) + \frac{1}{2} \left( \sum_{j_1,j_2} (Q_k^n)_{i,j_1,j_2}(x - x_k^n)_{j_1}(x - x_k^n)_{j_2} \right)_{i=0,1}
\]

with

\[
(Q_k^n)_{i,j_1,j_2} := \partial_{j_1,j_2}(\tilde{B}^n)_{i}(x_k^n)
\]
In practice: local approximation of the backward flows

- **Forward Jacobian**: approximate \( J_{k}^{n,\text{ex}} := J_{F_{k}}(x_{k}^{0}) \) with finite differences,
  \[
  J_{k}^{n} := \left( \frac{(\bar{F}^{n}(x_{k+e_{j}}^{0}) - \bar{F}^{n}(x_{k-e_{j}}^{0}))_{i}}{2h} \right)_{1 \leq i,j \leq d} = \left( \frac{(x_{k+e_{j}}^{n} - x_{k-e_{j}}^{n})_{i}}{2h} \right)_{1 \leq i,j \leq d}
  \]

- **Backward Jacobian**: using \( J_{B_{k}}(x_{k}^{n})J_{\bar{F}_{k}}(x_{k}^{0}) = I \), set
  \[
  D_{k}^{n} := (J_{k}^{n})^{-1}
  \]

- **Forward Hessian**: now approximate \( H_{k,i}^{n,\text{ex}} := H_{(F_{k})i}(x_{k}^{0}) \), \( 1 \leq i \leq d \), with
  \[
  H_{k,i}^{n} := (h)^{-2} \sum_{\alpha_{1},\alpha_{2}=0}^{1} (-1)^{\alpha_{1}+\alpha_{2}} (x_{k+\alpha_{1}e_{j_{1}}}^{n} + \alpha_{2}e_{j_{2}})_{i})_{1 \leq j_{1}, j_{2} \leq d}
  \]

- **Backward Hessian**: using \( 0 = (J_{k}^{n,\text{ex}})^{t} Q_{k,i}^{n,\text{ex}} J_{k}^{n,\text{ex}} + \sum_{l=1}^{d} (D_{k}^{n,\text{ex}})_l H_{k,l}^{n,\text{ex}} \), set
  \[
  Q_{k,i}^{n} := -(D_{k})^{t} \left( \sum_{l=1}^{d} (D_{k})_{i,l} H_{k,l}^{n} \right) D_{k}
  \]

- **Accuracy**: \( D_{k}^{n} = D_{k}^{n,\text{ex}} + \mathcal{O}(h^{2}), \quad Q_{k,i}^{n} = Q_{k,i}^{n,\text{ex}} + \mathcal{O}(h) \)
Polynomial particle transport: convergence estimates

Denote the backward flow error by

\[ e^n_{B,(r)}(h) := \sup_{k \in \mathbb{Z}^d} \| \tilde{B}_{h,k}^{n,(r)} - \tilde{B}^n \|_{L^\infty(\Sigma^n_{h,k})} \]

where \( \Sigma^n_{h,k} \approx \text{supp}(\varphi^n_{h,k}) \)

Theorem (MCP '14)

The LTP \((r = 1)\) and QTP \((r = 2)\) transport operators satisfy

\[
\|(T_r - T_{\text{ex}})f^0_h\|_{L^\infty} \lesssim \left(1 + \frac{e^n_{B,(1)}(h)}{h}\right)^d \frac{e^n_{B,(r)}(h)}{h}\|f^0\|_{L^\infty}
\]

for QTP particles restricted to domains of the form

\[
\Sigma^n_{h,k} := \tilde{F}^{n,(1)}_{h,k}(B_{\ell^n}(x^0_k, h\tilde{\rho}^n_{h,k})) \quad \text{with} \quad \tilde{\rho}^n_{h,k} := \rho^0 + \frac{1}{h} e^n_{B,(2),k}(h)
\]

Corollary

\[
\|(T_r - T_{\text{ex}})f^0_h\|_{L^\infty} \lesssim h^r C(F, r)\|f^0\|_{L^\infty}
\]

Proof: The backward flow errors satisfy

\[
e^n_{B,(r)}(h) \lesssim h^{r+1} |\bar{F}^n|_1^{r+1} |\tilde{B}^n|_{r+1}
\]
Numerical results: blob in Leveque’s flow

- **FSL**: slow convergence, lost at large remapping periods
- **LTP**: convergence improved for all remapping frequencies
- **QTP**: convergence improved for large remapping periods

\((L^\infty\text{ errors vs. number of particles, for different remapping periods)}\)
Numerical accuracy and robustness

- Final $L^\infty$ errors vs. average remapping period

From particles to hybrid semi-lagrangian

▶ see MCP (JSC '14)
Application to non-linear problems: 1D1V Vlasov-Poisson

Theorem (GH Cottet and PA Raviart, ’84)

Using fixed-shape particles, one has (with $t \leq T$ and $C = C(T)$)

$$ \| E_h(t) - E(t) \|_{L^\infty(\mathbb{R})} + \sup_{k \in \mathbb{Z}^2} \| Z_k^h(t) - F_{0,t}(z_k^0) \| \leq Ch $$

Theorem (MCP and F Charles, ’14)

Using LTP, there exists a constant $C = C(T)$ for which

$$ \| E_h^{n,*} - E(t_n + \frac{1}{2}) \|_{L^\infty(\mathbb{R})} + \sup_{k \in \mathbb{Z}^2} \| z_k^n - F_{0,t_n}(z_k^0) \| \leq C(h^2 + \Delta t^2) $$

holds for $n\Delta t \leq T$ (provided $\Delta t \lesssim \sqrt{h}$), moreover

$$ \| f_h^n - f_{ex}^n \|_{L^\infty(\mathbb{R}^2)} \leq C(h + h^{-1} \Delta t^2) $$

LTP method also applied with success to aggregation equations with F. Charles, JA Carillo and YP Choi
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Motivation: size matters!

(due to particle stretching, deposition on a grid becomes expensive, non-local)
New method based on local backward flows

- to every grid node $\xi_i = i h$, $i \in \mathbb{Z}^d$, we associate the closest particle $x^n_k$, 
  $$k = k^*(n, i) := \arg\min_k \|x^n_k - \xi_i\|$$
- define the corresponding local backward flow
  $$\bar{B}^{n,(1)}_{h,k} : x \mapsto x^0_k + D^n_k(x - x^n_k) \quad \text{with} \quad D^n_k \approx (J_{F^n_{ex}}(x^0_k))^{-1}$$
- option 1 (cheap try) : approximate $f^n(\xi_i)$ with 
  $$f^n_h(\xi_i) := f^n_h(\bar{B}^{n,(1)}_{h,k}(\xi_i)), \quad k = k^*(n, i)$$
- option 2 (almost as cheap) : with a partition of unity $\sum_i S_h(x - \xi_i) = 1$, let 
  $$\bar{B}^{n,(1)}_{h}(x) := \sum_i \bar{B}^{n,(1)}_{h,k^*(n,i)}(x)S_h(x - \xi_i)$$

and define the (L)-FBL approximation to $f^n$ as 
  $$f^n_h(x) := f^n_h(\bar{B}^{n,(1)}_{h}(x))$$
- same method works with quadratic flows...
FBL: convergence estimates

Theorem (MCP, F. Charles ’16)

The FBL approximations satisfy

\[ \| (T_{h,(r)} - T_{\text{ex}}) f_h^0 \|_{L^\infty} \lesssim e_{B,(r)}^n(h) \| f^0 \|_{L^\infty} \]

- again, \( e_{B,(r)}^n(h) := \sup_{k \in \mathbb{Z}^d} \| \tilde{B}_{h,k}^n(r) - \tilde{B}^n \|_{L^\infty(\Sigma_{h,k}^n)} \) with \( \Sigma_{h,k}^n = B_{\infty}(x_k^n, Ch) \)
- Reminder: the LTP (\( r = 1 \)) and QTP (\( r = 2 \)) approximations satisfy

\[ \| (T_{h,(r)} - T_{\text{ex}}) f_h^0 \|_{L^\infty} \lesssim \frac{e_{B,(r)}^n(h)}{h} \| f^0 \|_{L^\infty} \]

- Key argument: LTP/QTP estimates based on the bound

\[ |w_k| \| \varphi_h(\tilde{B}_{h,k}^n(r)(x)) - \varphi_h(\tilde{B}^n(x)) \| \leq |w_k| \| \varphi_h \|_{\text{Lip}} \| \tilde{B}_{h,k}^n(r) - \tilde{B}^n \|_{L^\infty} \lesssim \frac{e_{B,(r)}^n(h)}{h} \]

whereas for FBL we have

\[ \| f_h^0(\tilde{B}_{h}^{n,(1)}(x)) - f_h^0(\tilde{B}^n(x)) \| \leq |f_h^0|_{\text{Lip}} \| \tilde{B}_{h}^{n,(r)} - \tilde{B}^n \|_{L^\infty} \lesssim e_{B,(r)}^n(h) \]
Validation and comparison LTP/FBL

- Passive transport: blob in Leveque’s flow (RK4, $\Delta t = T/100$).

$L^2$ errors vs. $h$, for different remapping periods
Passive transport: smooth blob in Leveque’s flow
Passive transport: blob in simulated convection cell

- **LTP**
  - $D_l = 0.1$ (33 remappings)
  - $D_t = 0.5$ (5 remappings)
  - $D_t = 1.5$ (1 remapping)

- **QTP**
  - $D_l = 0.1$ (33 remappings)
  - $D_t = 0.5$ (5 remappings)
  - $D_t = 1.5$ (1 remapping)

- **LBFR**
  - $D_l = 0.1$ (33 remappings)
  - $D_t = 0.5$ (5 remappings)
  - $D_t = 1.5$ (1 remapping)

- **QBFR**
  - $D_l = 0.1$ (33 remappings)
  - $D_t = 0.5$ (5 remappings)
  - $D_t = 1.5$ (1 remapping)
Passive transport: affine density in non-linear rotation flow

From particles to hybrid semi-Lagrangian

Strasbourg, October 18
Two-stream instability (Vlasov-Poisson)

PIC with $128 \times 128$ or $512 \times 512$ grids, $t = 53$.
Remappings with LTP (left) or L-FBL (right)
CPU times: 3 s (low res), 16 s (high res LTP) and 10 s (high res L-FBL)
Philosophy?

From particles to hybrid semi-lagrangian
Summary

Music, when soft voices die,
Vibrates in the memory;

(Percy Bysshe Shelley)
Summary (expanded)

- New method to reconstruct a smooth, accurate density from existing particles.

Advantages compared to LTP/QTP:
- enhanced locality (critical in high dimensions, already significant in 2D for second order flows)
- improved convergence rates, less oscillations
- second order method (QBF) straightforward to define and implement

References
- MCP (JSC 2014) Towards smooth particles methods without smoothing
- MCP, E. Sonnendrücker, A. Friedman, S. Lund, D. Grote (JCP 2014) Noiseless Vlasov-Poisson simulations with linearly transformed particles
- MCP, F. Charles (SINUM 2016) Uniform convergence of a linearly transformed particle method for the Vlasov-Poisson system

Future steps:
- unstructured, adaptive markers
- extensions to other models and larger codes (Selalib platform)