Backward Lagrangian approximations with Forward particles

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acknowledgments to Stephane Colombi (IAP)

Freefem days

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Outline

1. One motivation and a few perspectives
2. The forward-backward lagrangian (FBL) method
3. Estimates and numerical results

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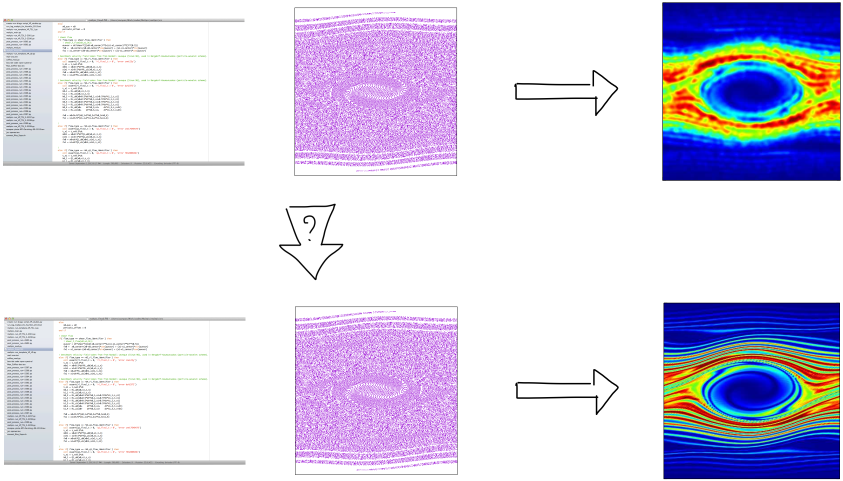
Main motivation : improvement of existing particle codes



Classical approaches to particle denoising

- represent f with smooth particle shapes φ_ε

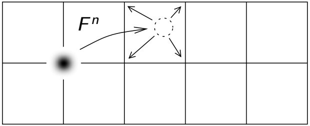
$$f^n_{h,\varepsilon}(x) = \sum_{k\in\mathbb{Z}^d} w_k \varphi_\varepsilon(x - x^n_k), \qquad \begin{cases} x^n_k : \text{particle center, pushed along fwd flow } F^n \\ \varepsilon : \text{particle size}, \quad hk \sim x^0_k \end{cases}$$

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

$$\|f^n_{h,\varepsilon} - f^n\|_{L^\infty} \le \sup_x |\langle f^n_h - f^n, \psi_{x,\varepsilon}\rangle| + \|f^n * \varphi_\varepsilon - f^n\|_{L^\infty} \lesssim \left(\frac{h}{\varepsilon}\right)^2 + \varepsilon^2$$

  - 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

A few perspectives

- Denoise an existing particle code
- Transform an existing particle code into an hybrid characteristic method
- Exploit a particular transport flow structure
- Implement in FreeFem++ ?

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A reconstruction method based on local backward flows

- to every grid node $\xi_i = ih$, $i \in \mathbb{Z}^d$, we associate the closest particle x_k^n,

$$k = k^*(n,i) := \mathrm{argmin}_k \|x_k^n - \xi_i\|$$

- define the corresponding local bacwkard flow

$$\bar{B}_{h,k}^{n,(1)} : x \mapsto x_k^0 + D_k^n(x - x_k^n) \qquad \text{with} \qquad D_k^n \approx \big(J_{\bar{F}^n_{\mathrm{ex}}}(x_k^0)\big)^{-1}$$

- option 1 (cheap try) : approximate $f^n(\xi_i)$ with

$$f_h^n(\xi_i) := f_h^0(\bar{B}_{h,k}^{n,(1)}(\xi_i)), \qquad k = k^*(n,i)$$

- option 2 (almost as cheap) : with a partition of unity $\sum_i S_h(x - \xi_i) = 1$, let

$$\bar{B}_h^{n,(1)}(x) := \sum_i \bar{B}_{h,k^*(n,i)}^{n,(1)}(x) S_h(x - \xi_i)$$

  and define the (L)-FBL approximation to f^n as

$$f_h^n(x) := f_h^0(\bar{B}_h^{n,(1)}(x))$$

- not a kernel smoothing

Approximate backward flows (1)

- principle : close to the particle x_k^n, approximate

$$\bar{B}^n(x) \approx \bar{B}_{h,k}^{n,(r)}(x)$$

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

$$\bar{B}_{h,k}^{n,(0)}(x) := x_k^0 + (x - x_k^n) \qquad \text{with} \qquad x_k^n := \bar{F}^n(x_k^0)$$

- order r = 1 (LTP) : use

$$\bar{B}_{h,k}^{n,(1)}(x) := x_k^0 + D_k^n(x - x_k^n) \qquad \text{with} \qquad (D_k^n)_{i,j} := \partial_j(\bar{B}^n)_i(x_k^n)$$

- order r = 2 (QTP) : use

$$\bar{B}_{h,k}^{n,(2)}(x) := x_k^0 + D_k^n(x - x_k^n) + \frac{1}{2}\Big(\sum_{j_1,j_2}(Q_k^n)_{i,j_1,j_2}(x - x_k^n)_{j_1}(x - x_k^n)_{j_2}\Big)_{i=0,1}$$

with

$$(Q_k^n)_{i,j_1,j_2} := \partial_{j_1,j_2}(\bar{B}^n)_i(x_k^n)$$

Approximate backward flows (2)

- Forward Jacobian : approximate $J_k^{n,\mathrm{ex}} := J_{\bar{F}^n}(x_k^0)$ with finite differences,

$$J_k^n := \left(\frac{(\bar{F}^n(x^0_{k+e_j}) - \bar{F}^n(x^0_{k-e_j}))_i}{2h} \right)_{1 \le i,j \le d} = \left(\frac{(x^n_{k+e_j} - x^n_{k-e_j})_i}{2h} \right)_{1 \le i,j \le d}$$

- Backward Jacobian : using $J_{\bar{B}^n}(x_k^n) J_{\bar{F}^n}(x_k^0) = I$, set

$$D_k^n := (J_k^n)^{-1}$$

- Forward Hessian : now approximate $H_{k,i}^{n,\mathrm{ex}} := H_{(\bar{F}^n)_i}(x_k^0)$, $1 \le i \le d$, with

$$H_{k,i}^n := \left((h)^{-2} \sum_{\alpha_1,\alpha_2=0}^{1} (-1)^{\alpha_1+\alpha_2} \left(x^n_{k+\alpha_1 e_{j_1} + \alpha_2 e_{j_2}} \right)_i \right)_{1 \le j_1, j_2 \le d}$$

- Backward Hessian : using $0 = (J_k^{n,\mathrm{ex}})^t Q_{k,i}^{n,\mathrm{ex}} J_k^{n,\mathrm{ex}} + \sum_{l=1}^d (D_k^{n,\mathrm{ex}})_l H_{k,l}^{n,\mathrm{ex}}$, set

$$Q_{k,i}^n := -(D_k^n)^t \left(\sum_{l=1}^d (D_k^n)_{i,l} H_{k,l}^n \right) D_k^n$$

- accuracy : $D_k^n = D_k^{n,\mathrm{ex}} + \mathcal{O}(h^2)$, $Q_{k,i}^n = Q_{k,i}^{n,\mathrm{ex}} + \mathcal{O}(h)$

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FBL : convergence estimates

Theorem (MCP, F. Charles '16)

The FBL appproximations satisfy

$$\|(T_{h,(r)} - T_{\rm ex})f_h^0\|_{L^\infty} \lesssim e^n_{B,(r)}(h)\|f^0\|_{L^\infty}$$

- here, $e^n_{B,(r)}(h) := \sup_{k\in\mathbb{Z}^d}\|\bar{B}^{n,(r)}_{h,k} - \bar{B}^n\|_{L^\infty(\Sigma^n_{h,k})}$ with $\Sigma^n_{h,k} = B_\infty(x^n_k, Ch)$
- with smooth particle reconstructions, (FSL, LTP, QTP...) we have

$$\|(T_{h,(r)} - T_{\rm ex})f_h^0\|_{L^\infty} \lesssim \frac{e^n_{B,(r)}(h)}{h}\|f^0\|_{L^\infty}$$

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

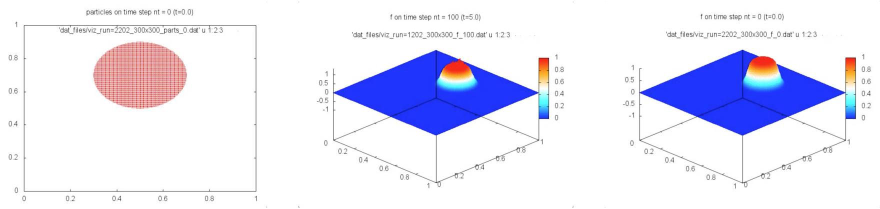
$$|w_k|\|\varphi_h(\bar{B}^{n,(r)}_{h,k}(x)) - \varphi_h(\bar{B}^n(x))\| \le |w_k||\varphi_h|_{\rm Lip}\|\bar{B}^{n,(r)}_{h,k} - \bar{B}^n\|_{L^\infty} \lesssim \frac{e^n_{B,(r)}(h)}{h}$$

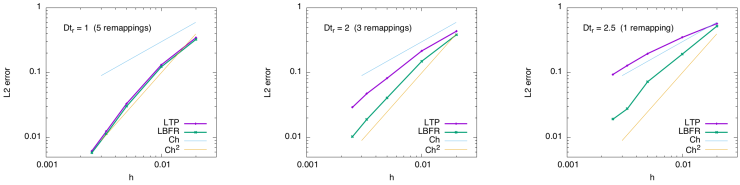
whereas for FBL we have

$$\|f_h^0(\bar{B}^{n,(1)}_h(x)) - f_h^0(\bar{B}^n(x))\| \le |f_h^0|_{\rm Lip}\|\bar{B}^{n,(r)}_h - \bar{B}^n\|_{L^\infty} \lesssim e^n_{B,(r)}(h)$$

Validation and comparison LTP/FBL

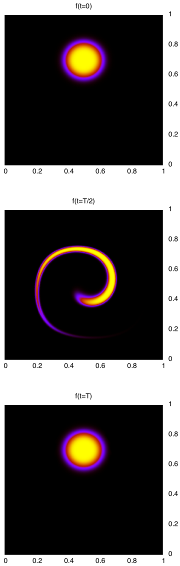
- Passive transport : blob in Leveque's flow (RK4, $\Delta t = T/100$).

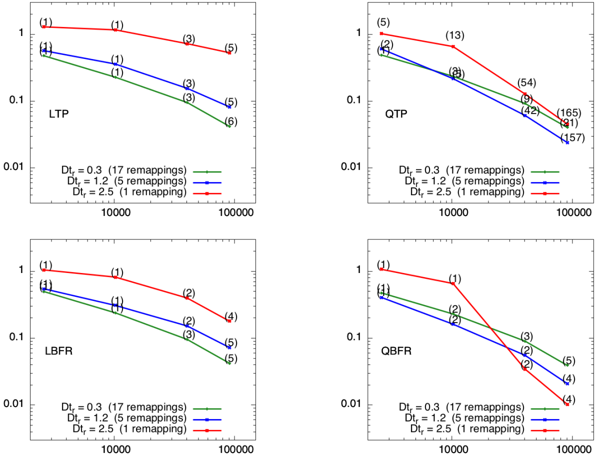




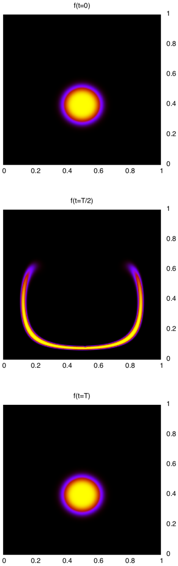
(L^2 errors vs. h, for different remapping periods)

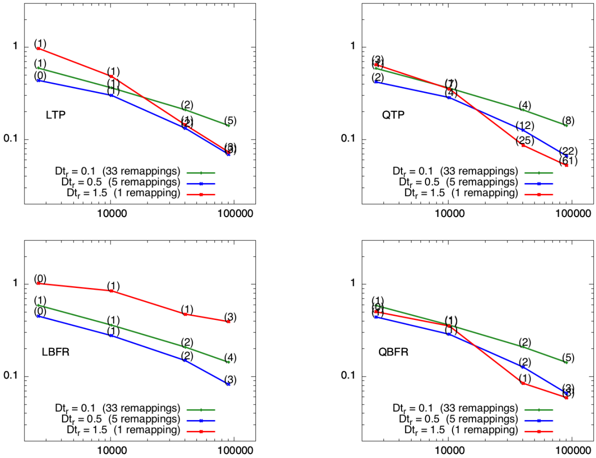
Passive transport : smooth blob in Leveque's flow



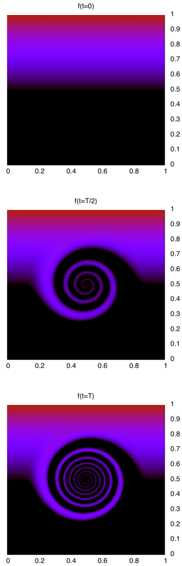


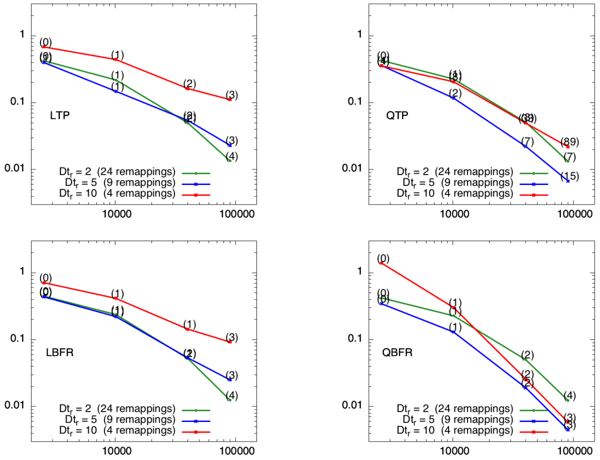
Passive transport : blob in simulated convection cell



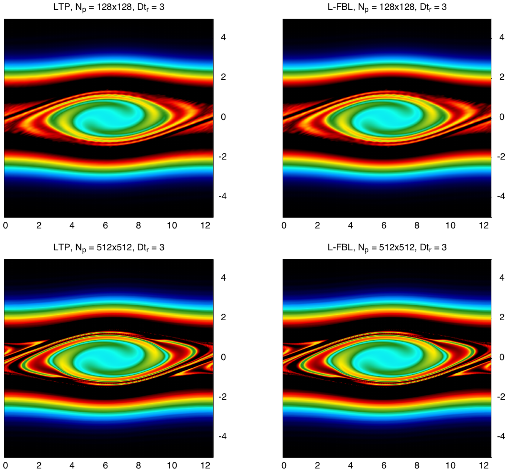


Passive transport : affine density in non-linear rotation flow



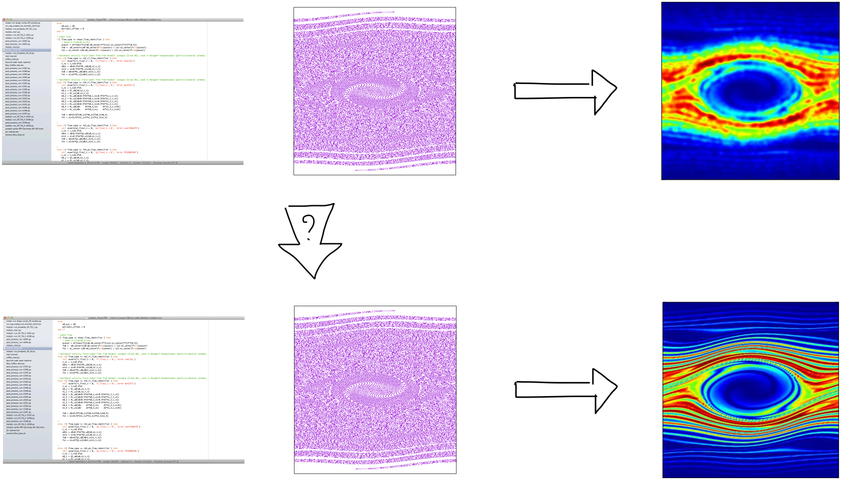


Two-stream instability (Vlasov-Poisson)



PIC with 128×128 or 512×512 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 ?



Summary

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

(Percy Bysshe Shelley)

Summary

Music, when soft particles 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, F. Charles (preprint)
    From particle methods to forward-backward Lagrangian schemes
  - S. Colombi (Vlasovia talk + preprint to appear soon)
- Future steps :
  - unstructured, adaptive markers
  - extensions to other models and larger codes (Selalib platform)