

# Semi-Lagrangian particle methods for complex fluid and fluid-structure dynamics 

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## Methods

- Multilevel, Semi-Lagrangian particle methods
- Immersed boundary technics for fluid-structure interactions

Applications

- Turbulent transport of passive and active scalars
- Simulation and optimization of flows around complex bodies

Issues

- Accuracy
- Flexibility
- Computational efficiency and parallel scalability

Outline
-Turbulent transport (I)
-Semi-Lagrangian particle methods

- Immersed boundary methods for fish optimization
-Multi-resolution semi-lagrangian particles
-Turbulent transport (II)
-Computational issues and hybrid computing

Accurate simulations of turbulent transport of scalar are of great importance in many applications


A $50 \times 100 \times 50$ smoke simulation with eight turbulence bands added to synthesize an effective resolution of $12800 \times 2560 \times 12800$


Tech achievement Oscar goes to Canadian software developers

The Canadian Pross Posted: Jan 4, 2013 9:43 AM ET | Last Updated: Jan 4, 2013 6:04 PMET


The team's Oscar-winning Wavelet Turbulence soffware is employed by visual effects artists to control the appearance of
smoke and gas on film. It has been used in big-budget movies ilke Battleship. (Universal Pictures/Associated Press)

## Equations of turbulent transport of a passive scalar:

Incompressible
Navier-Stokes equations

$$
\frac{\partial \vec{u}}{\partial t}+\vec{u} \cdot \vec{\nabla} \vec{u}=\vec{\nabla} \cdot(\nu \vec{\nabla} \vec{u})+\vec{\nabla} p, \vec{\nabla} \cdot \vec{u}=0
$$

$$
\frac{\partial \theta}{\partial t}+\vec{u} \cdot \vec{\nabla} \theta=\vec{\nabla} \cdot(\kappa \vec{\nabla} \theta)
$$

with appropriate boundary conditions

The ratio of fluid viscosity to scalar diffusivity is called the Schmidt number: $\mathrm{Sc}=\boldsymbol{v} / \boldsymbol{\kappa}$

## Challenge in DNS of turbulent transport:

Observation and theoretical prediction: depending on the value of Sc, energetic scales for scalar can extend far beyond those of the momentum (the Kolmogorov scale), with a «slow» $\mathbf{k}^{-1}$ decay

## Challenging numerical question:

$\checkmark$ How to resolve in an affordable way the significant scales in the scalar
$\checkmark$ Scaling of the scalar spectrum at the smallest scales?


Natural idea: decouple spatial resolutions for momentum and for scalar

$$
\Delta x^{\theta} \simeq \frac{\Delta x^{u}}{\sqrt{S c}} \Rightarrow N^{\theta} \simeq \sqrt{S c} N^{u}
$$

which solvers to choose for Navier-Stokes and transport equations?
$\Rightarrow$ Turbulent flow :
Spectral (periodic «academic» geometries) or Finite Volume (complex «engineering» geometries)
$\Rightarrow$ Scalar equation:
we need a method which

- is conservative
- is high order accurate (spectral-like)
- has good parallel scalability
$\bullet$ limits as much as possible the computational overhead
-> choice of Lagrangian or Semi-Lagrangian method :
- well adapted to transport equations
- time-step will not be constrained by very fine scalar mesh size

Particle methods with remeshing at every time-step can be viewed and analyzed as forward semi-lagrangian methods

How they work:
I) particles on a grid
2) push particles with local velocity values
3) remesh particles on the grid, through interpolation

In I D method can be described by the following equations:

$$
x_{i}^{n+1}=x_{i}+\tilde{u}_{i}^{n} \Delta t \quad \theta_{i}^{n+1}=\sum_{j} \theta_{j}^{n} \Gamma\left(\frac{x_{j}^{n+1}-x_{i}}{\Delta x^{\theta}}\right), i \in \mathbb{Z}^{d}
$$

where $\tilde{u}_{i}^{n}$ depend on the time-stepping scheme and $\Gamma$ is a piecewise polynomial kernel
$\Gamma$ is defined by regularity and moment properties :
A moment properties

$$
\sum_{k \in \mathbb{Z}} k^{\alpha} \Gamma(x-k)=x^{\alpha}, 0 \leq \alpha \leq p, x \in \mathbb{R}
$$

regularity :
$\Gamma$ is of class $C^{r}$ and $\Gamma \in \mathcal{C}^{\infty}(] l, l+1[), l \in \mathbb{Z}$
interpolation property: $\quad \Gamma(i)=\left\{\begin{array}{l}1 \text { if } i=0, \\ 0 \text { otherwise } .\end{array}\right.$

Convergence result (Cottet et al, M2AN 2014) :

1) the spatial order of the method is inf( $p, r$ )
2) stability holds for a large class of kernels under the condition $\Delta t \leq\|\vec{\nabla} \vec{u}\|_{\infty}^{-1}$

Remark : $\Delta t \leq\|\vec{\nabla} \vec{u}\|_{\infty}^{-1}$ is sometimes called a Lagrangian CFL condition (LCFL) with LCFL 1

## Examples of remeshing kernels (2nd and 6th order)

$$
\Lambda_{4,2}(x)= \begin{cases}1-\frac{5}{4}|x|^{2}-\frac{35}{12}|x|^{3}+\frac{21}{4}|x|^{4}-\frac{25}{12}|x|^{5} & 0 \leqslant|x|<1 \\ -4+\frac{75}{4}|x|-\frac{245}{8}|x|^{2}+\frac{545}{24}|x|^{3}-\frac{63}{8}|x|^{4}+\frac{25}{24}|x|^{5} & 1 \leqslant|x|<2 \\ 18-\frac{153}{4}|x|+\frac{255}{8}|x|^{2}-\frac{313}{24}|x|^{3}+\frac{21}{8}|x|^{4}-\frac{5}{24}|x|^{5} & 2 \leqslant|x|<3 \\ 0 & 3 \leq|x|\end{cases}
$$

$$
\Lambda_{6,6}(x)=\left\{\begin{array}{r}
1-\frac{49}{36}|x|^{2}+\frac{7}{18}|x|^{4}-\frac{1}{36}|x|^{6}-\frac{46109}{144}|x|^{7}+\left.\left.\frac{81361}{48}\right|^{2}\right|^{8}-\frac{544705}{144}|x|^{9}+\frac{655039}{144}|x|^{10} \\
-\frac{223531}{72}|x|^{11}+\frac{81991}{72}|x|^{12}-\frac{6307}{36}|x|^{13},
\end{array}, \quad 0 \leqslant|x|<1\right.
$$

Accuracy assessment : case of a rotating patch in an off-center vorticity field

$$
\boldsymbol{u}(x, t)=2 \cos (\pi t / T)\binom{-\sin ^{2}(\pi x) \sin (\pi y) \cos (\pi y)}{\sin ^{2}(\pi y) \sin (\pi x) \cos (\pi x)}
$$




Error in maximum norm for different kernels (order 1_2, 2_4 and 4_6)

## 3D case : comparisons with Weno and VOF methods

Implementation of grid-based methods with particles for corrections


Enright et al, JCP 2002 Vincent et al, JCP 2010

$3 r$ order Weno $\mathrm{N}=100+64 \mathrm{ppc}$

CFL=1 (?) CPU =??
$N=100, C F L=8$
$\mathrm{N}=160, \mathrm{CFL}=12$
CPU time :
$1 s$ per iteration
remeshed particle method, 4th order remeshing, 2nd order in time

$N=256$ and $C F L=30$. Left picture: kernel $\Lambda_{2,1} ;$ right picture: kernel $\Lambda_{8,4}$.

## Illustration of accuracy of the Semi-Lagrangian method compared to a spectral method

Scalar spectra given by spectral vs spectral/particle method in a decaying THI experiment with $\mathrm{Sc}_{\mathrm{c}}=50, \mathrm{~N}_{\mathrm{u}}=256, \mathrm{~N}_{\theta}=1024$
Particle method uses second order kernel


## Additional diagnostics


pdf of scalar gradient
 time evolution of scalar flatness

time evolution of scalar skewness


Forced homogeneous turbulence:
Systematic quantitative study of spectra at large, intermediate and small scales for a wide range of Reynolds and Schmidt numbers

Samples of simulations performed during the CTR Summer Program 2012 (on up to 8000 cores with MPI)

- Ratio of scalar/momentum resolution roughly given by $\mathrm{Sc}^{1 / 2}$
- Stability condition is independent of $\Delta x^{Z}$
- Case $R_{\lambda}=80$ and $S c=16$ established mixing dynamic takes 18 h instead of $\approx 12$ days with full spectral method.

| $R_{\lambda}$ | $N^{u}$ | $K_{\text {max }}^{u} \eta_{K}$ | $\Delta t^{u}$ | Sc | $N^{\theta}$ | $K_{\text {max }}^{\theta} \eta_{B}$ | $\Delta t^{\theta}$ | $\Delta t_{\text {spec }}^{\theta}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 130 | $256^{3}$ | 1.73 | $1.2 \mathrm{e}^{-2}$ | 0.7 | $512^{3}$ | - |  | $6 \mathrm{e}^{-3}$ |
|  |  |  |  | 4 | $1024^{3}$ | 3.39 |  | $3 \mathrm{e}^{-3}$ |
|  |  |  |  | 8 | $1024^{3}$ | 2.45 |  | $3 \mathrm{e}^{-3}$ |
|  |  |  |  | 16 | $1536{ }^{3}$ | 2.61 | $8.6 \mathrm{e}^{-2}$ | $2 \mathrm{e}^{-3}$ |
|  |  |  |  | 32 | $1536{ }^{3}$ | 1.85 |  | $2 \mathrm{e}^{-3}$ |
|  |  |  |  | 64 | $2048^{3}$ | 1.76 |  | $1.5 \mathrm{e}^{-3}$ |
|  |  |  |  | 128 | $3064{ }^{3}$ | 1.79 |  | $1 \mathrm{e}^{-3}$ |
| 210 | $512^{3}$ | 1.79 | $3 \mathrm{e}^{-3}$ | 0.7 | $770^{3}$ | - | $2 \mathrm{e}^{-2}$ | $2 \mathrm{e}^{-3}$ |
|  |  |  |  | 4 | $1024^{3}$ | 1.76 |  | $1.5 \mathrm{e}^{-3}$ |

Scaling of the large and intermediate scales


Scaling of smallest scales

$k \eta_{B}$
Laboratoire
JEAN KUNTZMANN

Scaling at large and intermediate scales Depending on Reynolds and Schmidt numbers, $k^{-5 / 3}$ or $k^{-1}$ or both scaling found in accordance with theoretical predictions

## Scaling at the smallest scales

Numerical results in good agreement with Kraichnan's theory: $k^{-1} \exp (\alpha . k)$

## Example of jet simulation using one billion particles for the scalar on 8 GPUs at $\mathbf{1} \mathbf{f p s}$ $\operatorname{Re}=10^{4}, \mathrm{Sc}=10$


side view
top view

# Handling complex geometries and Fluid-Structure Interactions with Immersed boundary technics 

Regular (Cartesian) grid with your (favorite) Navier-Stokes solver


No-slip boundary conditions Elastic stresses



Application to the 3D simulation and optimization of swimming
Conventional approach would use body-fitted FV methods, ALE mesh generation and coupling boundary conditions between fluid and body


Fluid-solid interface coupling and interface conditions

Body-fitted mesh generation
Time consuming and difficult to extend to several bodies
Alternative approach based on penalization method in cartesian grids
I) Penalization method for one-way interaction [Angot-Bruneau-Fabrie 1999]
-S the rigid body at a given time, subject to gravity forces, embedded in a computational box $\Omega$

- ū = prescribed body velocity,
- $\mathrm{X}_{\mathrm{s}}=\mathrm{I}$ in the body, 0 outside and
- $\lambda$ a (large) penalization parameter
then :

$$
\rho\left(\frac{\partial u}{\partial t}+(u \cdot \nabla) u\right)-\nu \Delta u+\nabla p=\rho g+\lambda \rho \chi_{S}(\bar{u}-u) \quad \text { in the computational box } \Omega
$$

> + boundary conditions (e.g. periodic)
2) extension to two-way interaction [Coquerelle, C. 2008; Bost, C., Maitre 2009]: computation of solid velocities not prescribed but obtained by projection of flow velocity onto rigid body velocity:

$$
\overline{\bar{u}=\frac{1}{|S|} \int_{K} \chi_{S} u d x+\left(J^{-1} \int_{K} \chi_{S} u \times\left(x-x_{G}\right) d x\right) \times\left(x-x_{G}\right)}
$$

where $J$ is the inertia matrix of the body $K$, and $\mathrm{XG}_{\mathrm{G}}$ is its mass center.

S is captured by a level set function, advected with the rigid motion $\bar{u}$ :

$$
\frac{\partial \phi}{\partial t}+(\overline{\mathbf{u}} \cdot \boldsymbol{\nabla}) \phi=0
$$

In practice: solid motion allows to compute $\phi$ analytically
3) In a vorticity formulation, leads to

$$
\frac{\partial \omega}{\partial t}+(u \cdot \nabla) \omega-(\omega \cdot \nabla) u-\nu \Delta \omega=+\lambda \nabla \times \chi_{S}(\bar{u}-u) .
$$

complemented by the usual system giving $u$ from $\omega$, and the coupling of $\bar{u}$ with the flow and the contact forces
4) Extension to deforming bodies (Gazzola et al. 201I)

$$
\bar{u}=u^{t}+u^{r}+u^{\text {translation }}={ }^{\text {rotation }} \underset{ }{\substack{\text { deformation } \\ \\ \\ \\ \\ \text { result of body-flow interaction }}}
$$

- Penalization methods offer flexibility and reduce computational cost, but at the expense of lower accuracy near the boundaries
- Requires to locally refine in adaptive manner

At each time-step, wavelet-based MRA of (grid) quantities, based on interpolating wavelets :

$$
q(\boldsymbol{x})=\sum_{\boldsymbol{k} \in \mathcal{K}^{0}} c_{\boldsymbol{k}}^{0} \varphi_{\boldsymbol{k}}^{0}(\boldsymbol{x})+\sum_{l=0}^{L-1} \sum_{\boldsymbol{k} \in \mathcal{K}^{l}} \sum_{\mu=1}^{2^{d}-1} d_{\boldsymbol{k}}^{l, \mu} \psi_{\boldsymbol{k}}^{l, \mu}(\boldsymbol{x})
$$

where $d$ is the dimension and scaling functions and wavelets are recursively given by filter operations

$$
\varphi_{\boldsymbol{j}}^{l}=\sum_{\boldsymbol{k}} H_{\boldsymbol{j}, \boldsymbol{k}}^{l} \varphi_{\boldsymbol{k}}^{l+1}, \quad \psi_{\boldsymbol{j}}^{l, \mu}=\sum_{\boldsymbol{k}} G_{\boldsymbol{j}, \boldsymbol{k}}^{l, \mu} \varphi_{\boldsymbol{k}}^{l+1}
$$

basis functions for scales spaces $\mathcal{V}^{l}$ at level $l$ and $l+1$
basis functions for details spaces $\mathcal{W}^{l}$ at level $l$ and $l+1$

$$
\mathcal{V}^{l+1}=\mathcal{V}^{l} \bigoplus \mathcal{W}^{l}
$$

Nested grids and grid adaptation based on thresholding detail coefficient (Liandrat \& Tchamitchian, 1990,Vasilyev 2003)

Particle method advects/remeshes scale solution at the successive scales, level by level, then combine results to reconstruct solution and perform MRA for next iteration

Nested grids, for wavelet coefficient above given threshold : $\quad\left\{\mathcal{K}_{>}^{l}\right\}_{l=0}^{L}$
An additional buffer is created around particles activated at level $l$, with values obtained by interpolation from level $l-I$, to allow consistent remeshing

$$
\boldsymbol{\mathcal { B }}^{l}=\left\{\boldsymbol{k}^{\prime}\left|\min _{\boldsymbol{k} \in \mathcal{K}_{>}^{l}}\right| \boldsymbol{k}^{\prime}-\boldsymbol{k} \left\lvert\, \leq\left\lceil\frac{1}{2} \operatorname{supp}(\zeta)+\mathrm{LCFL}\right\rceil\right.\right\}
$$

Finally, like for grid-based methods, need to allow levels $l+\mid$ to appear from level $l$ during advection step. Important: time steps given by LCFL $=1$ are ok: time scale on which scale $l+1$ appear from scale $l$ is given by $d t_{l \rightarrow l+1}=\ln 2 /|\nabla u|$

## Algorithm for time advancement of particles at a given level $l$



a
select «active» particles on the grid (with $\mathrm{tag}=1$ )

$$
\underline{u(x)}
$$


advect particles and tag
d

remesh particles and tag; keep particles with tag >0

## Back to the stretching-by-rotation patch

$$
\boldsymbol{u}(x, t)=2 \cos (\pi t / T)\binom{-\sin ^{2}(\pi x) \sin (\pi y) \cos (\pi y)}{\sin ^{2}(\pi y) \sin (\pi x) \cos (\pi x)}
$$

error in area enclosed by contour at time $\mathrm{T}=8$


Number of active particles or grid points at time $t=0$ and $t=8$

Illustration of particle MRA for flow around a wind turbine (ETH group of Koumoutsakos)
Ingredients : wavelet-based particles for vorticity transport and
Brinkman penalization for non-slip boundary conditions (Angot et al., I999, Coquerelle \& Cottet, 2008)


## 3D anguilliform swimming




## C-start is an escape motion pattern

## Is C-start optimal?



Preparatory stroke


Muller, van den Boogaart, van Leeuwen. J. of Exp.Biology, 2008.

FLOW @ $R e=\frac{L^{2} / T_{\text {prop }}}{\nu}=550$

## 4.4mm long larva zebrafish of age 5 days post-fertilization

## GEOMETRY


$\begin{array}{ccccc}\text { PARAMETERS } & \left.\kappa_{s}(s, t)=B(s)\right) f\left(\frac{t}{T_{\mathrm{p} r e p}+T_{\mathrm{p} r o p}}\right) & +K(s)) \sin \left[2 \pi\left(\frac{t}{T_{\mathrm{prop}}}-\tau(s)+\phi\right]\right. \\ 8 & = & 3 & +1 & +1\end{array}$


## Optimization strategy : evolutionary algorithm + covariance matrix adaptation <br> C-start is OUTCOME of optimization





Pros and cons of the Wavelet-based multi-resolution particle method
Pros:

- great compression / efficiency boundary layer / wake
- well adapted to Lagrangian transport of scales

Cons:

- Scalability non optimal, load balancing difficult (not a problem for evolutionary optimization)
- In a vorticity particle method, velocities of particles have to be recovered through Biot-Savart lax and Fast Multipole solver.

$$
\mathbf{u}\left(\mathbf{x}_{p}\right)=\sum_{q \neq p} v_{q} \omega_{\mathbf{q}} \mathbf{K}\left(\mathbf{x}_{q}-\mathbf{x}_{p}\right)
$$

Much more expensive than FFT-based Poisson solvers

Alternative (more naive approach) : Bi-level formulation of vorticity transport

3D Euler equations in vorticity formulation $\frac{\partial \boldsymbol{\omega}}{\partial t}+\operatorname{div}(\mathbf{u} \boldsymbol{\omega})-[\nabla \mathbf{u}] \boldsymbol{\omega}=0$
Using higher resolution for vorticity than for velocity is equivalent to advecting vorticity with mollified velocity

$$
\frac{\partial \boldsymbol{\omega}}{\partial t}+\operatorname{div}(\overline{\mathbf{u}} \boldsymbol{\omega})-[\nabla \overline{\mathbf{u}}] \boldsymbol{\omega}=0
$$

where $\operatorname{div} \bar{u}=0, \operatorname{curl} \bar{u}=\bar{\omega}$, and $\bar{\omega}=\omega^{*} \zeta_{\varepsilon}$
In practice means that

- $\omega$ computed (advection-diffusion equation) on fine grid
$\bullet \bar{u}$ computed on coarse grid, from filtered field $\bar{\omega}$

Problem : these modified NS equations induce enstrophy production at the sub-grid scale

This can be analyzed and overcome by appropriate "minimal" nonlinear dissipation terms [C., JCP 1996]

This is reminiscent to subgrid-scale models involved in Large Eddy simulations

To compensate for this backscatter, need to introduce anisotropic subgridscale dissipation :

$$
\frac{\partial \omega}{\partial t}(x)=C \int[\omega(x)-\omega(y)][(u(x)-u(y)) \cdot \nabla \zeta(x-y)]_{-} d y
$$

with linear cut-off, easily discretized on a 27-points stencil.

Constant C needs to be tuned (unfortunately)

## Proof of concept on Taylor-Green vortex

[C. Mimeau, PhD thesis 2015]

$$
\begin{aligned}
& u_{x}(\mathbf{x}, t=0)=\frac{2}{\sqrt{3}} \sin \left(\theta+\frac{2 \pi}{3}\right) \sin (x) \cos (y) \cos (z) \\
& u_{y}(\mathbf{x}, t=0)=\frac{2}{\sqrt{3}} \sin \left(\theta-\frac{2 \pi}{3}\right) \cos (x) \sin (y) \cos (z) \\
& u_{z}(\mathbf{x}, t=0)=\frac{2}{\sqrt{3}} \sin (\theta) \cos (x) \cos (y) \sin (z)
\end{aligned}
$$

Comparison of enstrophy in a fully resolved
$512^{3}$ simulation [van Rees et al., JCP 2011] and in a bi-level $64^{3} / 256^{3}$ simulation


Case without subgrid-scale dissipation and unphysical enstrophy growth


Case with subgrid- ${ }^{\top}$ cale dissipation with $\mathrm{C}=0.04$

Temporal evolution of enstrophy

## Contours of vorticity in a cross-section


$128^{3} / 512^{3}$ simulation
$512^{3}$ simulation
(van Rees et al., JCP 2011)

Similar results with turbulent plane jets (with same value of coefficient C)

What is the point of doing of using different particle resolution for velocity and vorticity (is there any CPU gain at all)?

Vorticity advancement implies only local operations (advection - remeshing -diffusion)
-> good parallel scalability
Velocity calculation implies non-local operations (Poisson solver, FFT ..) : fast but not highly parallel

## Hybrid computing idea :

- distribute operation intensive parallel parts of the algorithm (vorticity) to GPU (or accelerators)
- keep less operation intensive (more communication demanding) on classical CPU.

Proof of concept of transport of passive scalar:
Summary of performance for hybrid CPU /GPU implementations of
Navier Stokes / scalar transport


> Performance equivalent to conventional MPI implementation of same method on several thousand Blue Gene cores

Ongoing : extension to Navier-Stokes (transport of vorticity) DNS at the price of a LES ?

## Conclusion and outlook

SL Particle methods combined with immersed boundary technics efficient in many CFD problems dominated by transport

## Efficiency relies on

-high order algorithms, not constrained by CFL conditions
$\bullet$-ability to be combined with grid-based technics, including MRA
-high parallel scalability

## Ongoing works:

- explore double-diffusion at high Sc with hybrid method, in Finite Volume NS solvers
- continue the validation of the vorticity/velocity bi-resolution approach on turbulent jets and boundary layers
- implement it on hybrid architectures
- extend the approach to (finite-difference,velocity-pressure)/(particles,level set)
for multiphase flows with surface tension, using new semi-implicit time-discretization [CottetMaitre, JCP 2016]

