Lagrangian methods in fluids and combustion

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Abstract

Lagrangian, mostly grid-free methods, offer natural approaches to simulate convection, adaptively, while avoiding diffusive errors. They have been extended successfully to finite Reynolds number flows, low Mach number combustion, and high Mach number flows. This presentation summarizes the essential elements of Lagrangian, grid-free methods, and demonstrates their applications in a number of nonreacting and reacting flows of canonical and practical interest.

Keywords: Lagrangian methods; Vortex and particle methods; Smooth particle hydrodynamics; Fluid flow, Combustion

1. Introduction

Grid-free, particle-based Lagrangian methods rely on kernel representation to approximate flow variables; quadrature rules to approximate resulting integrals; take advantage of conservation properties along particle trajectories, and utilize moment preserving redistribution of particle strength to simulate diffusion [1]. Boundary conditions require special treatment, e.g. vorticity generation on no-slip boundaries [2] and a zero flux condition to enforce no penetration [3]. Implementation for different flow conditions, including reacting and compressible flows, is summarized next. The method demonstrates superior performance in cases of unsteady and unstable, unconfined flows, flows with concentrated, evolving vorticity and sharp gradients, and high Reynolds number multi-scale flows.

2. Inviscid methods

The vortex method was originally conceived as an efficient way to model the short time evolution of a vortex sheet [4]. Many years later, the method was revived and extended to smooth flows by replacing singular vortices with elements of finite support, or kernels. Analysis suggested that the convergence rate depends on the structure of the kernel, and the degree of overlap of neighboring vortices, showing that the element core radius must be larger that the distance between the centers of neighboring elements [5]. In this representation, a continuous vorticity field is represented as

$$\omega(x,t) = \sum_{i=1}^{N} \alpha_i(t) f_\delta(x - \chi_i(t)) \tag{1}$$

where $\alpha_i = (\omega \mathrm{d}V)_i(t)$ is the total vorticity associated with an element of volume $\mathrm{d}V$ and vorticity vector ω, x,t are location vector and time, respectively, χ_i is the instantaneous location of an element and N is the number of elements. $f_\delta = \delta^{-3} f\left(\frac{|r|}{\delta}\right)$ is the normalized kernel function, it is an approximation of the Delta function to a given order. The condition of overlap pointed to the need to increase the number of elements in flows in which strong strains magnify the distance between elements. Furthermore, the distortion of the vortex element distribution due to the evolution of a complex flow map was recognized as another source for possible deterioration of the long time accuracy that should be overcome by mapping elements over a more uniform distribution every so often. Interpolation formulae that do so with minimum numerical errors were developed [1].

The open space velocity field induced by the vorticity distribution in Eq. (1) is given by the following summation:

$$u_\sigma = \sum K_\delta \alpha_i \tag{2}$$

where $K_\delta = K^* f_\delta$, and K is the Green's function of the Laplacian. Vorticity stretch in 3-D is computed

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explicitly by updating the local vorticity vector according to the velocity gradient, evaluated by differentiating the velocity field, leading to the following finite dimensional representation of the flow:

$$\frac{\mathrm{d}\chi_i}{\mathrm{d}t} = u_i$$

and

$$\frac{\mathrm{d}\alpha_i}{\mathrm{d}t} = \alpha_i.\nabla u \tag{3}$$

Figure 1 shows an example for the application of the inviscid method, in terms of the results of a simulation of vortex breakdown using vortex filaments, that is connected space curves of vorticity, to model the initial distribution of vorticity, the formation of a recirculation zone and wavy wake structure [6].

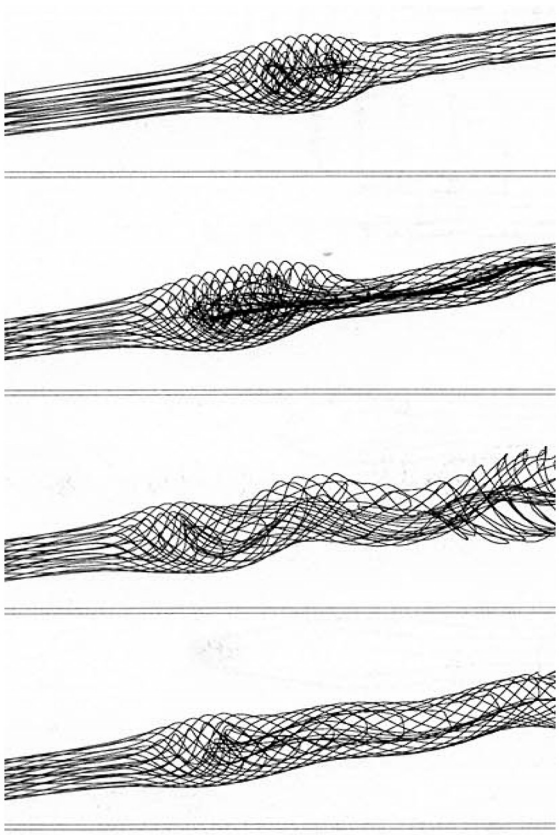

Fig. 1. Simulation of vortex breakdown. The flow in the original streamwise vortex is moving toward the right and spinning in a counterclockwise direction, circulation number = 3.52. Results show the formation of a recirculation zone followed by a wavy wake. The figure shows the time evolution of the vortex filaments from the time of the breakdown onward.

3. Viscous flow

Viscous flow simulation was first suggested using random walk methods, in which convection is augmented by a displacement drawn from a statistical distribution whose properties depend on the dimensionality, Reynolds number, and time step. The method, albeit noisy, proved successful in capturing interesting dynamics [2,3]. Figure 2 shows results of a simulation of the operation of a two-stroke, opposed piston engine using a three dimensional vortex code.

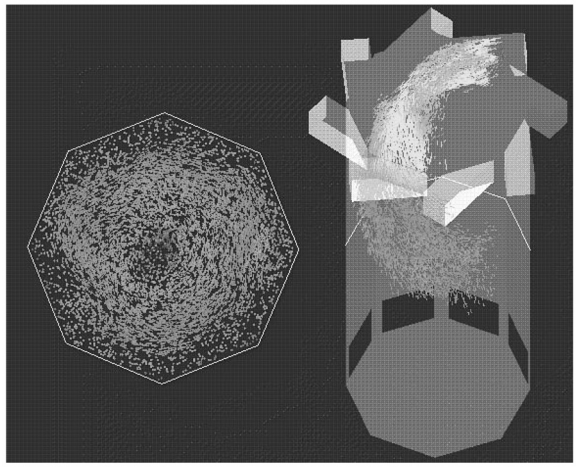

Fig. 2. Simulation of the intake process in an opposed piston engine. The RHS shows a perspective of the engine cylinder with intake ports at top and exhaust ports at bottom, and the flow elements entering from one port only are shown for clarity. The LHS shows a cut halfway between top and bottom, showing the swirling motion inside the cylinder.

Deterministic methods formulated next were based on the concept of core expansion, in which the local solution of a viscous vortex is used to model the diffusion of the global vorticity field. For instance, in 2-D, if the core function is a second-order Gaussian, then the core expands according to

$$\delta^2(t + \Delta t = \delta^2(t) + 4\nu\Delta t \tag{4}$$

where ν is the diffusivity. Several modifications to improve the accuracy, essentially amounting to dividing each growing element into a number of smaller ones while preserving some vorticity moments, were later suggested.

A number of schemes that rely on the exchange of the vorticity carried by each element among itself and the neighboring elements were formulated later. In one approach, an integral approximation of the diffusion equation is the starting point:

$$\nabla^2\omega(x) = \frac{2}{\delta^2}\int (\omega(y) - \omega(x))\eta_\delta(y - x)dy \qquad (5)$$

where the function η approximates the kernel of the diffusion equation [7,8]. This approach preserves the identity of the elements, while changing their strength, and hence the name 'particle strength exchange', or PSE, and adds more elements immediately outside the support of the exiting volume of elements to capture the ever expanding support of vorticity due to diffusion. The integral is approximated by a quadrature and the resulting ODEs are integrated to update the vorticity of the elements.

Another redistribution approach, by matching the moments of the exact solution of a diffusing vortex with those generated by a local distribution, was formulated in [9]. Posed as a Galerkin approximation of the diffusion equation, the method can be generalized to arbitrary diffusivity and dimensionality. The method was extended recently to ensure the regularity of the elements at all times by choosing the target elements in the diffusion step to lie on a regular mesh [10]. This method was used to simulate a transverse jet at Re = 1750, and the results are shown in Fig. 3. Results demonstrate the ability of the method to capture the breakdown of the vorticity structure and the generation of small scales. Both the particle exchange and the redistribution methods apply to flows with variable diffusivity.

4. Fast methods

The velocity field computation requires the performance of an N-body interaction problem, and, at sufficiently large number of elements, the cost can be prohibitive. Fast summation methods have been formulated on the basis of clustering particles according to some criterion, and replacing particle–particle interactions with cluster–particle or cluster–cluster interactions. A recursive tree structure is typically used in subdividing the domain, and the influence of a cluster is computed using higher order expansions of the particle field to reduce the errors while allowing larger clusters to be used at the leaf cells. Typically, multipole expansion of the velocity kernel is used, but other expansions have also been suggested. More recently, Taylor series expansion of the desingularized kernel was used, with recursive relations to evaluate the higher order term, as well as adaptive cell construction [11]. Yet another advancement involved the application of k-means clustering to achieve optimal domain decomposition for the purpose of parallelizing that algorithm [12].

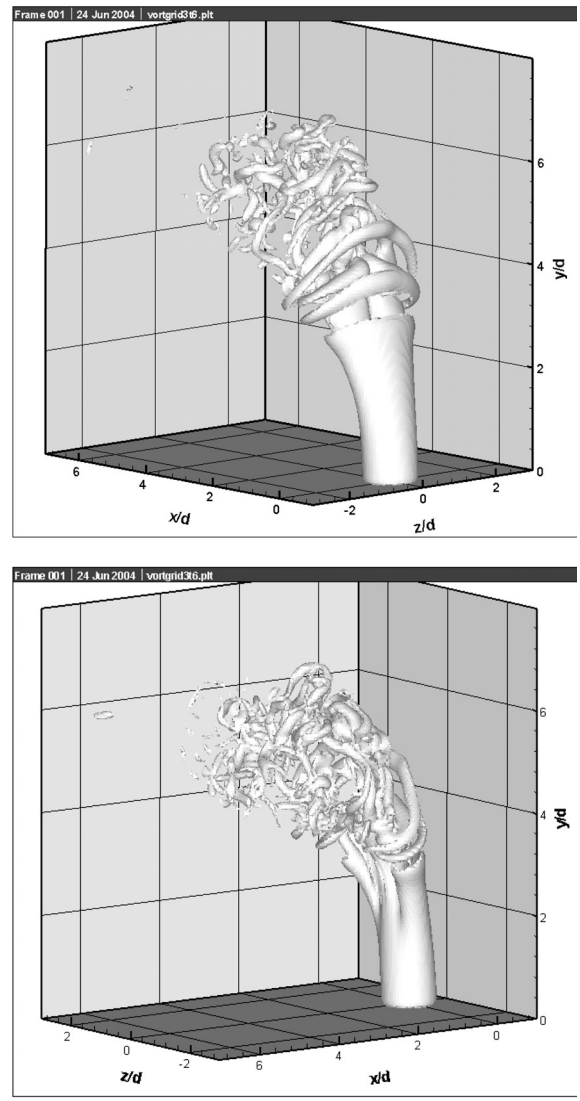

Fig. 3. Simulation of a transverse jet. Vorticity isosurface at $|\omega| = 20$ and $t = 6.0$. (*a*) View from the upstream side showing delayed Kelvin-Helmholtz instability; (*b*) View from the downstream side showing counter-rotating vortex pairs. All results were obtained from the case at $\mathrm{Re}_{\mathrm{jet}} = 1715$ and $r = 7$.

5. Low Mach number combustion

In combustion, the coupled continuity, momentum, energy, and chemical species transport equations must be solved simultaneously to model the tight coupling between the combustion-induced flow, and the impact of flow-induced transport on the combustion processes. Combustion-induced flow is represented by a velocity divergence, which is proportional to the Largangian derivative of the density, and a vorticity source whose

magnitude is proportional to the products of the pressure and density gradient. Borrowing from the ideas of the vortex method, gradients of the density, temperature, etc., can be transported along particle trajectories, thus eliminating the need for elements where uniform conditions exist [13,14]. Equations governing gradient transport have been used for that purpose, and approximations relating the gradient evolution to flow kinematics have been used to simplify the analysis. Results in Fig. 4 show the structure of a reacting shear layer in terms of the vortex elements, vorticity, and products distributions.

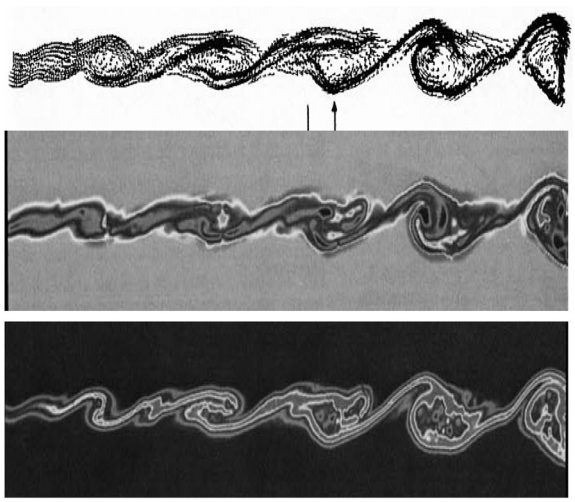

Fig. 4. Simulation of a reacting shear layer, with fuel on the upper side and air on the lower side. The top figure shows all the computational elements used in the simulation, the middle figure shows the vorticity distribution, and the bottom figure shows the product's concentration/temperature distribution.

In other developments, fluid elements transporting density, energy and chemical species are used around areas of non-zero gradients. The functional representation of these variables resembles that expressed in Eq. (1). Their convective and diffusive transports are done in the same way as that of the vorticity, while the chemical source terms are integrated to change the local strength of the elements [15,16].

6. High Mach number flow

While vortex methods use the vorticity as the primary variable transported by Lagrangian particles, and compute velocity by summing over the fields of the vortices, smoothed particle hydrodynamics, or SPH, methods transport primitive variables, that is the velocity field, besides the enthalpy, density, and other gas dynamic variables [17]. The method uses reproducing kernels to evaluate the derivatives in the governing equations, and updating the Lagrangian variables. The method has been successful in inviscid compressible flow applications and more recently has been extended to viscous compressible flow by treating the viscous terms using approaches similar to PSE methods. Reactive flow simulations were performed using SPH, in which the chemical source terms are integrated along the particle trajectories [18]. In another development, the vortex method was extended to simulate compressible flows at arbitrary Mach numbers by transporting, along with the vorticity, the local dilatation, which is updated using a transport equation derived by taking the divergence of the Navier-Stokes equations [19]. Flow derivatives were computed using an extension of the PSE method. Moving least squares, in which local interpolation functions are developed and used to get derivatives required in the governing equations, have been used by others for the same purpose. In these methods, similar to the partition of unity, the interpolation window moves to cover the neighborhood of the area where derivatives are being evaluated

7. Looking ahead

The natural adaptivity of Lagrangian methods provides optimal distribution of the computational elements and hence minimizes the work required in volume gridding, adaptive meshes and moving boundaries. With the current state of the art, it is possible to perform direct simulations of complex flows.

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