Contribution to the modeling of complex physical systems described by PDE[1]: a 2D multi-agent model for convection-diffusion

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We propose here a multi-agent approach to simulate transport phenomena described by PDEs. The agents-particle are inspired by particle elements (volume or mass) of particle methods such Smoothed Particle Hydrodynamics. They have with their autonomy, vicinity perception, capacity of rearrangement and evaluation of their mutual contribution. In order to compare our multi-agent system with the classical models, we implement a model in Netlogo (a multi-agent platform) to simulate the convection-diffusion transport in two dimensions.

[1]Partial Differential Equations

1 Introduction

Partial differential equations (PDEs) are widely used in the numerical simulation of linear or non-linear, stationary or dynamic, laminar or turbulent physical systems. Numerical grid-based methods such as the finite element method (FEM) or the finite difference method (FDM) were widely applied these last decades and remain most popular. However, these methods suffer from some limitations (difficulties on irregular or complex geometry for the FDM and on mesh distortion or large deformation problems for the FEM). This led to the development of meshfree and particle methods [Li 2002] that are more efficient because they use a Lagrangian[2] approach (SPH: Smooth Particle Hydrodynamics [Monaghan 1985], Element Free Galerkin [Belytschko 1994], Vortex methods [Cottet 2000], [Liu 2005]...). Nevertheless, the particle methods still have limits in the management of the particle behavior when submitted to complex boundary conditions, and in the approximations through quadrature points because of particles irregular repartition. Until now, there is not a numerical method which is better than all others on all aspects, while the studied problems become more and more complex and hard to represent (impact penetration, explosion, fluid-structure interactions, sediments transport, erosion...).

$$\frac{\partial u}{\partial t} + V.\nabla u - D\Delta u = 0 \tag{1}$$

The convection-diffusion described by (1) is the basic transport process for a wide range of physical, biological and chemical processes. Some examples are:

- the evolution of the concentration field $u(x,t)$ of a material (a pollutant or tracer with diffusivity D) in a fluid with velocity V,
- the evolution of the vorticity field $u(x,t)$ in a turbulent flow where V is also the velocity field and D the kinematic vorticity. (Vortex methods for the Navier-Stokes velocity-vorticity equation),
- heat transfers (diffusion equations).

In this phenomenon, the material is transported (convection) while diffusing in the same time. Convection dominates diffusion in most cases (i.e. high Peclet[3] number). This generates, in a grid-based method resolution, a numerical dispersion or an oscillatory scheme (added to already seen limitations!). There are fortunately stable and numerical-dispersion-free lagrangian methods, for high Peclet number, as random walk or Particle Strength-Exchange but they also have their drawbacks. The first method has difficulties in handling boundary conditions and introduces errors because of its stochastic nature (the diffusion process is treated in a random way). The second one needs frequent remeshing of particles positions because it uses these positions as quadrature points to approximate the Laplacian (or the differential diffusion operator). "The particle adaptation comes at the expense of the regularity of the particle distribution as particles move in order to adapt to the gradients of the flow field" [Bergdorf 2005]. The irregularity causes accuracy loss in the quadratures.

[2] The material is represented by a set of moving particles. The field quantities are reconstructed by a linear superposition of the individual fields carried by particles

[3] $Pe = |V| / D$, similar to Reynolds number in fluid dynamics

After relating all these difficulties in numerical simulation, we can notice that for dynamic physical systems, such mass or heat transport, fluid flow... it would be interesting, for improving existing lagrangian approaches, to endow virtual particles of some (individual or collective) capacities in order to surpass some specific limits. We propose for that an agent-particle approach in which particles have:

- vicinity perception and adaptive behavior mechanisms (to handle some complex boundary conditions, and to optimize time computing)
- capacity of rearrangement and evaluation of their mutual contribution (for functions approximations).

An outline of the paper is as follows. We first recall in section 2 the numerical simulation procedure. SPH that is the basis of our model is also briefly presented as a particle method in section 3. In section 4, the multi-agent particle approach is discussed. The convection-diffusion is finally implemented in section 5 with the Netlogo agent-based platform. This will allow us to review initial and boundary conditions, kernel approximations, adaptive particle core radius…

2 Numerical simulation and PDE-based models

To obtain a mathematical model for the simulation of physical systems, some characteristics as the velocity, the height, the pressure…(fluids); the displacement and constraints (elasticity problem); the concentration (transport problem) are taken as continuous time- (and/or space-) dependant variables. Applying on these selected variables conservation's laws of mass, energy, momentum… one can obtain governing equations of systems in the form of a PDE set. There are numerous complex systems governing equations. In physics: Poisson and Laplace's equation for stationary phenomenon, heat equation for evolution phenomenon, wave equation for propagating phenomenon, Korteweg-de Vries equation for waves on shallow water surfaces, Schrödinger equation in non-relativistic quantum mechanics, Navier-Stokes equation for incompressible viscous fluids… In biology and chemistry, Turing's reaction-diffusion equation for morphogenesis phenomenon and in population dynamics, Von Foerster equation… For most physical systems an analytical resolution is quasi-impossible, they have to be resolved in a numerical way (space and time discretization). For a complete review of numerical methods, you can refer to: [Euvrard 1990], [Li 2002], [Belytschko 1996].

3 A particle method: the SPH

Originally defined for astrophysical problems, the SPH method has been well specified by [Monaghan 1985] and is now widely applied. Given N particles P_i of mass m_i (or other characteristic) in a domain Ω, SPH uses particle positions x_i as quadratures points in order to approximate with (2) any field function f (density, pressure, viscosity…) and its derivatives. m_i/φ_i is the elementary volume, W the smoothing kernel and h the core radius (Fig. 1).

$$< f(x) >= \int_\Omega f(y)W(x-y,h)dy \quad \Rightarrow \quad < f(x) >\approx \sum_{i=1}^{N} f_i.\frac{m_i}{\varphi_i} W(x-x_i,h) \qquad (2)$$

We use in this paper the 2D kernel functions (3): W_C (*cubic B-spline*) and W_P (*Poly6*), where $r = \|x - x_i\| / h'$, $s = \|x - x_i\|$ and $h' = h/2$.

$$W_C(r,h') = \frac{10}{7\pi (h')^2} \begin{cases} 1 - \frac{3}{2} r^2 + \frac{3}{4} r^3 & r < 1 \\ \frac{1}{4} [2 - r]^3 & 1 \le r < 2 \\ 0 & 2 \le r \end{cases}, \quad W_P(s,h) = \frac{4}{\pi h^8} \begin{cases} (h^2 - s^2)^3 & s \le h \\ 0 & otherwise \end{cases} \tag{3}$$

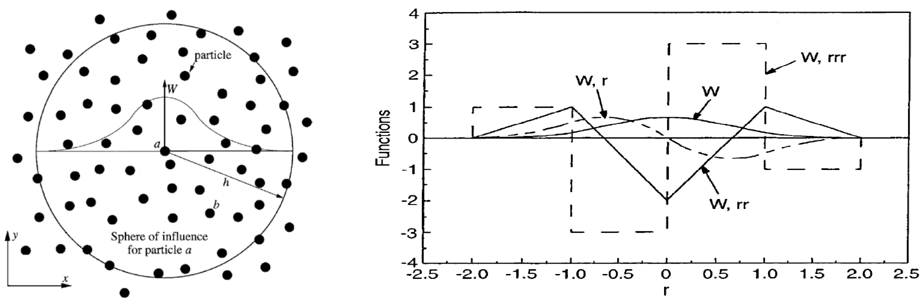

Figure. 1: The SPH influence zone of a particle *a*, and the distributions of the cubic B-spline function W and its first three derivatives (W, r W, rr and W, rrr).

4 From the particle to the agent

Notice that another weakness of particle methods is in the way of resolving equations of motion (in a dynamic system). Those methods have to rewrite equations (set of EDPs) in a Lagrangian formulation and to express them by a set of ODEs using approximation (2). After that, they will integrate the obtained ODEs, to numerically resolve equations of motion. The algebraic resulting system is then too closed to implement some improving actions (or behaviours) on particles.

Thus, in our approach, particles are not considered only as virtual entities driven according to satisfaction rules of governing equations but also as autonomous. The autonomy isn't in the physical behaviour[4], but in the perception of environment/neighbours and in actions resulting of decisional interactions rules (aggregation, dislocation, messages exchanging...). Using agent-particles can allow in the simulation to handle the particle methods already seen difficulties or to implement others improvements. Multi-agents systems have already been used in fluid dynamics context [Servat 2000], [Bertelle 2000] and show good promises.

4.1 The modeling procedure

In our multi-agent model, we'll find first steps of the numerical simulation procedure until to the domain discretization step. After that, we consider each particle

[4] Particles are of course submitted to external forces

individually (as agent-particle) to drive it. Fig. 2 illustrates the general evolution of the proposed agent-particle (according to the modelled problem, the graph states may change). We'll come back on the core radius updating, the function approximations and others concepts (Laplacian operator, interaction/influence/perception zone…) in the convection-diffusion problem.

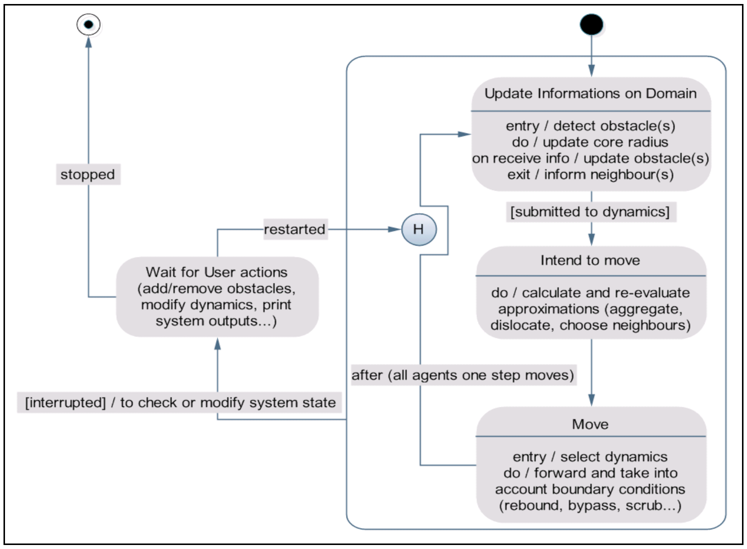

Figure. 2: UML State Diagram of an agent-particle in a dynamic system

We also decide to introduce in the model an agent-domain (observer in Netlogo) to generate initial conditions. The agent-domain may also manage boundary conditions (Dirichlet condition: production or disappearance of material, Neumann condition: flow condition on normal boundary direction…) and alert the system about new obstacles and dynamics conditions changes.

5 The convection-diffusion

The convection-diffusion transport is performed in two phases; particles are advected according to the fluid field velocity (in convection phase) and particles naturally diffuse (the diffusion phase). The first phase is trivial when the field velocity is well defined. In this study we treat the diffusion phase by determining the diffusion velocity [Degond 1990]. In fact we can rewrite the diffusion equation in (4). The diffusion becomes then similar to advection according to the velocity A that depends to the density. We so have to find good density approximations.

$$0 = \frac{\partial u}{\partial t} - D\Delta u = \frac{\partial u}{\partial t} - D\nabla(A.u) \;\text{ with } A = \frac{\nabla u}{u} \tag{4}$$

5.1 The interaction/influence zone

In SPH, the smoothing length h_a (the interaction/influence zone) of a particle a must be updated[5] during the simulation process in order to keep the number of interacting particles roughly constant and to obtain good approximations (25 to 30 particles in 2D). When changing the interactions zone, one has to take into account anti-symmetrical contribution between particles. For two interacting particles, that means the contribution calculated with the kernel W now depends on both interaction/influence zones (for more details refer to SPH documentation).

In a "space-oriented" multi-agent platform, especially Netlogo, we don't need structures (as ordered lists of particles locations that are used in particle methods) to deal with interacting particles. The agent-particle just has to ask at agent-domain (observer) his neighbourhood. Updating the interaction/influence zone is easier too and carried out with the old interacting/influence zone (which is an agent-particle attribute) and the current configuration.

5.2 Modeling the diffusion

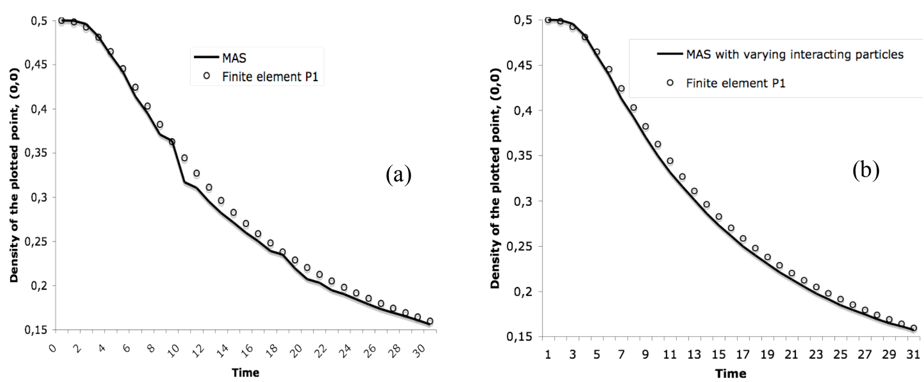

Figure. 3: Comparison between the multi-agent model and finite element method on diffusion

To test the diffusion phase of our model, we compare it to the finite element method (which can simulate simple-diffusion process) on a uniform density centred disk (Appendix A). We notice that in the beginning (fig. 3.a), the model shows good results but after several time steps loses accuracy even by maintaining the number of interacting particles. This is due to the fact that the number of interacting particles concerns uniform distributions. When noting relevant changes in the repartition of an agent and his neighbours during diffusion process, we should change the previous number of interacting particles to obtain better approximations. An agent-particle a can memorize and update a reference map of positions and during the simulation compare it to the maps generated by news positions in order to determine if the regularity is still kept. In the diffusion process (from an uniform repartition) a simple

[5] Smaller in high-density areas and larger in low-density areas.

way is to establish a comparison criterion based on linear combinations of vectors $\vec{r}_i = (\vec{x}_a - \vec{x}_i)/h$. Fig. 3.b shows the improvement obtained by varying the number of interacting particles.

To simulate the convection-diffusion problem, particles have to be first "advected" (supposing that convection dominates diffusion) and in the second phase, apply the diffusion process (or vice-versa)[6]. We obtain very good results in the approximation of the diffusion term (Laplacian operator) that is the main problem of particle methods. Nevertheless, improvements have to be made on the comparison between our multi-agents model and particle methods in others study cases.

5.3 Detecting coherent structures

An important issue in the study of complex dynamical systems may be the detection of coherent structures in the materiel (or the environment) during the evolution, in order to establish different levels of description of the phenomenon. This can be useful, either for the optimization of time computing, or for the understanding of the "beta-levels" of the studied phenomena (example: detecting and following vortical structures in turbulent fluid). An agent-based model can help in that way, not just by localizing iso-values or historic correlations (in the relevant fields functions), but also by generating new beta-agents and providing the discovered beta-interactions which can give an upper view of the system. Fig 4. gives an example of generated agents based upon the density field evolution of the rotating disk (a convection diffusion with the following parameters for the velocity field: $\vec{v}_x = \vec{y}$, $\vec{v}_y = -\vec{x}$)

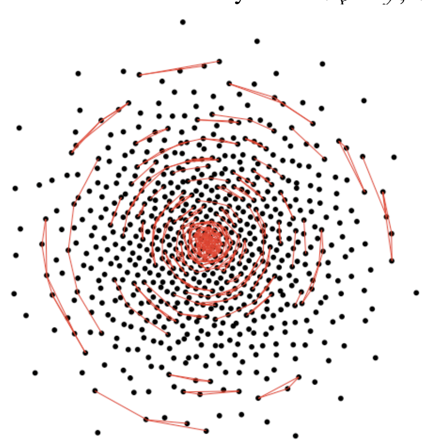

Figure. 4: Virtual agents (in red) appearing from a convection-diffusion (rotating) disk

6 Conclusion

The principal contribution of multi-agents systems, for particles methods, in this context of physical complex systems described by PDE, is the autonomy of the particles, their perception and their adaptation mechanisms. They offer an open

[6] Find our Netlogo online program at: http://sma-dynasys.freehostia.com

framework to take into account more and more complex geometries and boundary conditions. Multi-agent systems are then able to constitute an evolution, or a logical continuation of the particles methods used in numerical simulation. They may bring other improvements in the functions approximation procedure, and in the detection of coherent structures in flows in order to move easily between relevant levels of description in such complex systems.

Bibliography

[1] T. Belytschko, Y. Y. Lu, and L. Gu, "Element free Galerkin methods" International Journal for Numerical Methods in Engineering, vol. 37, pp. 229–256, 1994.

[2] T. Belytschko, Y. Krongauz, D. Organ, M. Fleming, M. P. Krysl, Meshless methods: An overview and recent developments. Computer Methods in Applied Mechanics and Engineering, Vol. 139, pp. 3-47,1996.

[3] M. Bergdorf, G.-H. Cottet & P. Koumoutsakos , Multilevel Adaptive Particle Methods for Convection-Diffusion Equations, SIAM Multiscale Modeling and Simulation, 4, 328-357, 2005.

[4] C. Bertelle, D. Olivier, V. Jay, P. Tranouez et A. Cardon, A multi-agent systeme integrating vortex methods for fluid flow computation, 16th IMACS Congress 2000, Vol. 122-3, Lausanne, Switzerland, 21-25 Août 2000

[5] G.H. Cottet, P. Koumoutsakos, Vortex Methods: Theory and Practice. Cambridge Univ. Press, Cambridge, UK. ,2000.

[6] P. Degond and F. J. Mustieles, A deterministic approximation of diffusion equations using particles, SIAM J. Sci. Stat. Comput. 11(2), 293 (1990).

[7] D. Euvrard, Résolution numérique des équations aux dérivées partielles de la physique, de la mécanique et des sciences de l'ingénieur : Différences finies, éléments finis, méthode des singularités. 2ème édition. Masson. 1990.

[8] S. Li, W. K. Liu, Meshfree and Particle Methods and Their Applications. Applied Mechanics Review, Vol. 55, pp 1-34, 2002

[9] Liu G. R. and Liu M. B., Smoothed particle hydrodynamics: a meshfree particle method, World Scientific, 2003.

[10] L. Liu, F. Ji, J. Fan, K. Cen, Recent development of vortex method in incompressible viscous bluff body flows. Journal of Zhejiang University Science. Vol. 6A No. 4 pp 283-288, 2005.

[11] J. J. Monaghan, Particle methods for hydrodynamics. Comput. Phys. Rep. 3, 71–124, 1985.

[12] D. Servat, Modélisation de dynamiques de flux par agents. Application aux processus de ruissellement, infiltration et érosion. Thèse de Doctorat. Université Paris 6, 2000.