Lattice Boltzmann Method for Ocean Oil Spill Propagation Model and Simulation:

A Comparison Study of Navier-Stokes Model and Advection Diffusion Model

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Outline

- Ocean oil spills and their devastating impacts
- The fate of spilled oil in ocean and its transport.
- Lattice Boltzmann Method (LBM) as a kinetic based model for ocean oil spill
- LBM Model and Simulation Benchmarks

- > LBM Model with Ocean Current
- Comparison of LBM Advectiondiffusion Equation (ADE) and Naiver-Stokes Equation (NSE)
- Conclusion and Further Research.

Gulf of Mexico LBM ADE Oil Concentration Model

The domain of study area with UWIN-CM Ocean Model in Gulf of Mexico covers:

➢ longitude (-88.9 to -87.9)

> latitude (28.3 to 29.3)



Devastating Impact of Ocean Oil Spills



- > 2010 DWH Spill in Gulf of Mexico lasted 87 days.
- \succ It released over 3 million barrels of oil.
- > It impacted over 1,600 miles of coastline.

- > It killed over 8000 marine animals/seabirds.
- Estimated loss in tens of billions of dollars in fishing and tour industries.
- It impacts long-term public health and quality of life of millions of people.



The Fate of Spilled Oil in the Ocean



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i. After oil introduced into the oceans;ii. Transport the resulting degradation oil away from the source;

iii. Incorporate the residual substances into compartments of the earth's surface system



Ocean Oil Spill Transport

Modeling spilled oil transport is a complex process involves:

- Ocean surface currentWind
- > Temperature
- chemical composition of the oil and seawater



https://www.spf.org/en/_opri_media/profile/investigate/technology/img/technology06.jpg

Lattice Boltzmann Method (LBM)

- LBM is a kinetic theory based modeling technique.
- Modeling ocean oil pollutants as a set of particles with certain density and mass located on a lattice, X.
- Track particle spatial positions and microscopic momentum in discrete steps.
- A continuum of velocity directions and magnitudes and varying particle mass are reduced (in 2-D model, D2Q9) to 9 directions and a unit particle mass.



The LBM Equations and a Simulation Algorithm

Macroscopic fluid density and velocity:

 $\rho(X) = \sum_{a=0}^{8} f_a(X); \quad u(X) = \sum_{a=0}^{8} f_a(X) e_a$

For near incompressible fluids, an equilibrium distribution function f^{eq} is defined by Kruger as in [6]:

$$f_a^{eq}(X) = w_a \rho(X) \left[1 + \frac{3e_a u}{c^2} + \frac{9(e_a u)^2}{2c^4} - \frac{3u^2}{2c^2} \right]$$

were $w_a = \left[\frac{4}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36}, \frac{1}{36} \right]; \ a = 0 \ to \ 8.$

Streaming and collision of the particles via the distribution function:

 $\overline{f_a(X+e_a\Delta t,t}+\Delta t) =$

 $f_a(X,t) - [f_a(X,t) - f_a^{eq}(X,t)]/\tau;$

where τ is a relaxation time.

- A LBM simulation model can be implemented in a algorithm outlined by Bao et al [24]:
 - 1. Initialize ρ , u, f_a and f_a^{eq}
 - 2. Streaming step: move $f_a \rightarrow f_a^*$, in the direction of e_a
 - 3. Compute macroscopic ρ and u from f_a^* .
 - 4. Compute f_a^{eq}
 - 5. Collision step: calculate the updated distribution function :

 $f_a = f_a^* - (f_a^* - f_a^{eq}) / \tau$

Repeat step 2 to 5.

Note: f_a^* holds intermediate values that are used in the BGK operation.

Advantages of LBM Model

- LBM Model can provide numerical solutions for both Naiver-Stokes Equation (NSE) and Advection-Diffusion Equation (ADE).
- LBM is well suited to simulate multiphase/multicomponent flows.
- Complex boundaries are easier to deal with using on-grid bounce-back and thus LBM can be applied to simulate flows with complex geometries.
- LBM can be parallelized and thus can be applied to do large simulations.

LBM NSE Model Benchmark - Poiseuille Flow

*LBM NSE model is a 64 x 64 lattice with $\tau = 5.0$ and a steady force factor to drive the flow from left to right.

Boundary conditions:

- Double periodic bounce back (left and right walls)
- Halfway bounce back (top and bottom walls)
- Zou-He bounce back (top and bottom walls)





LBM Advection-Diffusion Equation (ADE) Model

 au_{g}

> The governing physical equations: $\frac{\partial u}{\partial t} + u\nabla u = -\frac{\nabla P}{\rho} + \nu\nabla^2 u + F \quad (NSE)$

$$\frac{\partial C}{\partial t} + u\nabla C = D\nabla^2 C + q \qquad (ADE)$$

- \succ LBM equations:
 - NSE

$$f_a(x + e_a\Delta t, t + \Delta t) = f_a(x, t) - \frac{[f_a(x, t) - f_a^{eq}(x, t)]}{\tau}$$

• ADE

$$g_a(x + e_a\Delta t, t + \Delta t) = g_a(x, t) - \frac{g_a(x, t) - g_a^{eq}(x, t)}{\tau_g}$$

> NSE conserves mass and momentum and ADE only conserves mass.

Table T. A list of numerical quantities in both models.		
LBM NSE Model	LBM ADE Model	
Calculate $\rho(x,t)$ and $u(x,t)$	Calculate C(x, t)	
Conserve mass and	Conserve mass	
momentum		
Kinematic viscosity,	Diffusion coefficient,	
$\nu = \frac{c^2}{9}(\tau - \frac{\Delta t}{2})$	$D = \frac{c^2}{9} (\tau_g - \frac{\Delta t}{2})$	
Relaxation time, $\tau = 5.0$	Relaxation time, τ_g =6.25	
D2Q9 lattice (512 by 512)	D2Q9 lattice (512 by 512)	
Lattice speed, $c=\Delta x/\Delta t$	Lattice speed, $c=\Delta x/\Delta t$	
Calculated velocity field, u	Specified velocity field, u	

imperiant quantities in both

LBM ADE Model Benchmark - Gaussian Hill

LBM ADE Model Configuration:

- > LBM ADE model with a 512 x 512 lattice
- We did a benchmark study of Gaussian Hill vs. the analytical solution, as well as, an ADE numerical solution based on a FDM Finite Differential Method (FDM).
- Gaussian Hill as an initial concentration distribution at location of (200, 200) of the lattice.

We used a uniform ocean surface velocity field as an advection velocity field, U = (u_x, u_y) = (0.10, 0.10)

The Gaussian Hill analytic solution:

- > Initial Gaussian Hill concentration $\frac{\left[(X-X_0-u_xt_0)^2+(Y-Y_0-u_yt_0)^2\right]}{2\sigma_0^2}$ $C(X,t_0) = C_0 e^{\frac{2\sigma_0^2}{2\sigma_0^2}}$
- Solution Gaussian Hill mass concentration at time t $C(X,t) = \frac{\sigma_0^2}{\sigma_0^2 + \sigma_D^0} C_0 e^{-\frac{\left[(X - X_0 - u_x t)^2 + (Y - Y_0 - u_y t)^2\right]}{2(\sigma_0^2 + \sigma_D^0)}}$

where diffusion coefficient D=1.5 specified and $\sigma_D = \sqrt{2Dt}$.

LBM ADE Benchmark - Gaussian Hill

Table 2: LBM ADE and FDM ADE parameter list			
LBM ADE	FDM ADE		
Lattice grid: 512 by 512	N=512, X=[1:N], Y=[1:N]		
Lattice velocity: $\Delta x / \Delta t = 1$	∆t = 1		
Relaxation time: τ_g =6.25	Kappa=1.5		
Initial Gaussian hill	Initial Gaussian hill		
location:	location:		
(X ₀ ,Y ₀)=(200,200)	(X ₀ , Y ₀)=(200, 200)		
Concentration $C_0 = 1$,	Concentration C ₀ = 1,		
$\sigma_0 = 10$	$\sigma_0 = 10$		
External velocity:	External velocity:		
$U=(u_x, u_y)=(0.10, 0.10)$	$U=(u_x, u_y)=(0.10, 0.10)$		







LBM ADE Model Benchmark - Gaussian Hill

> Maximum concentration over time



Impacts of τ_g values to diffusions at t=200

Method	C max	X max	Y max
Analytic	0.142820	220	220
FDM	0.142506	221	221
LBM (τ _g =6.25)	0.138113	218	218
LBM (_{tg} =6.00)	0.144020	217	217
LBM (τ _g =5.00)	0.174000	217	217

Dialled-in from 0.138 to 0.144 to approach the analytic solution of 0.143 by changing τ_g from 6.25 to 6.00.

LBM ADE Model Benchmark - Perturbed Taylor Green Velocity Field

- Using a temporal and spatial perturbation of the Taylor-Green velocity field
- A 2-D ADE model with a concentration field, C = C(x, y, t) and a fluid velocity field, $u = (u_x, u_y)$
- \succ The initial concentration is given as:

 $C_0 = C(x, y, t_0) = sin(x) over [-\pi, \pi]$

> A perturbed Taylor-Green flow as the fluid velocity field: $u = \begin{bmatrix} \sin(x)\cos(y) + \varepsilon(2\sin(x - \omega t)\cos(2y) - k) \\ -\cos(x)\sin(y) - \varepsilon\cos(x - \omega t)\sin(2y) \end{bmatrix}$

- Benchmark LBM ADE and FDM ADE over Perturbed Taylor Green Flow
- > FDM computation domain is a 256x256 lattice over $(-\pi, \pi)$ and $\Delta t = 0.001$
- > LBM Computation domain is a 256x256 lattice over (1, 256) and $\Delta t = 1.0$

LBM ADE and FDM ADE Taylor Green Solutions

- The LBM model is implement in both Python and MATLAB while the FDM model is implement in MATLAB.
- Both models are implemented with double periodic boundary conditions.
- Our benchmark results show both models agree closely.
- This study shows LBM ADE is suitable to model oil transport in a temporal-spatial depended ocean flow









LBM NSE and ADE Coupled Model with Gaussian Hill

- The LBM NSE model reveals that the Gaussian Hill collapses at the center after initial distribution and the mass propagate outwards in a ring form as shown in Fig. (a) and (b).
- While we do believe what Fig. (a) and (b) show is the correct numerical solution of the NSE solver, it is not a suitable model for ocean oil transport.
- We conducted an experiment to couple NES and ADE using NSE to solve mass and velocity then feed them to ADE as shown in Fig. (c) and (d).









(c) ADE Gaussian Hill after 0.2 second



(b) LBM NSE mass propagations at t=100 (d) ADE concentration after 0.2 second

A Comparison Study of LBM NSE and ADE with Ocean current Models

- LBM, as a kinetic modelling technique, is capable to provide numerical solutions for both NSE and ADE solvers.
- The major difference between the two models is that NSE conserves both mass and momentum while ADE only conserves mass.
- ADE is the most commonly used to model ocean oil spill and pollutant transports, there are little or no reported studies using NES for such applications
- What role NSE can play in modeling ocean oil spill?

- > Using UWIN-CM as an Ocean Current Model
- Using a linear interpolation method to generate a velocity field for the LBM model domain (a sub area of Gulf of Mexico)
- The ocean surface velocity filed is integrated in LBM NSE model using a velocity project schema described by [6]:

 $u = \frac{1}{\rho} \sum_{0}^{8} e_a f_a + \frac{F\Delta t}{2\rho}$

LBM ADE model uses the ocean velocity filed as an external adventive velocity.

LBM NES and ADE Model Configurations

- We used a subset of data from the ocean model to cover an area of Gulf of Mexico centered at (-88.4 longitude and 28.8 latitude) over three days (Feb. 08, 2016 to Feb. 10, 2016).
- > For proof of concept, we use a Gaussian hill representing oil spill with σ =10 and C_0 =0.1 and a backdrop of ocean water mass with C=1 uniformly.
- In a real oil spill application, these parameters need to be carefully calibrated according to the specify oil spill and the type of oil.

- Using a real ocean current model requires a careful consideration of spatial-temporal scales between the physical and the LBM models.
- For a stable numerical solution, we also scaled down the ocean velocity by 10⁻²

Table 5. Physical and LBM Spatial-Temporal Scales		
Physical Scale	LBM Scale	
A grid with 200x200 cells. Cell size 500m by 500m.	A lattice with 200 by 200 cells.	
Centered at (-88.4, 28.8)	Cell size. Lattice cell size: $\Delta x = \Delta y = 1$ Isu (lattice space unit)	
Duration 3 days start 07- Feb 2016 16:00 ∆t=15 m	$\Delta t = 1$ Itu (lattice time unit);	
Total steps: t=0 to 296	total steps: t=0 to 296	
Physical velocity: U _p =V _p =500m/900s=0.56m/s	Lattice velocity: $U_L=V_L=\Delta x/\Delta t=1 lsu/ltu;$	

Case Study #1 - LBM ADE with Ocean Model



ADE Mass C and velocity at t=0 step



ADE Mass C and velocity at t=96 step



ADE Mass C and velocity at t=296 step

Case Study #2 - LBM NSE with Ocean Model







NSE Mass C and velocity at t=0 step

NSE Mass C and velocity at t=96 step

NSE Mass C and velocity at t=296 step

Conclusion and Future Research

- Our study and simulation results show how a LBM can be a multi modal framework to model ocean oil spills in both NSE and ADE based models via Poiseuille flow and Gaussian hill benchmarks against analytic solutions.
- We benchmarked the LBM ADE with a perturbed Taylor Green flow and demonstrated that the LBM ADE can be a suitable model for oil transport in an ocean with a spatial-temporal depended flow.
- We compared LBM NSE and ADE models and found that NSE can play a role in tracking interactions between velocity generated by rapid mass redistribution and ocean current velocity at least during initial spill.

- We did a proof concept study to integrate ocean surface current velocity from a real ocean model into a LBM models (NSE and ADE).
- Further research on using drifter data that are available from CARTHE in their Lagrangian Sub mesoscale Experiment (LASER). To investigate feasible and suitable ways for assimilating drifter data into LBM models to improve accuracy of predicting oil transport for example in the Gulf of Mexico.
- Further research on using LBM model for multi-fluids in oil weathering process and to use LBM NSE to model the oil droplet formations in the mixture of oil and seawater.

Gulf of Mexico LBM ADE Oil Concentration Model with LDA3 Drifters - Future Work



Questions and Discussions

