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Computational Modeling of Fluid-Fluid Flows Employing Adaptive Mesh Refinement, Front-Tracking, Immersed Boundary and Volume-of-Fluid

Prof. Dr. Aristeu da Silveira Neto (UFU/FEMEC)



Work Team

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Infrastructure: MFLab



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Infrastructure: Cluster - MFLab



SGI ICE X e SGI Altix XE

- 2 racks e 54 nodes;
- Total numbers of cores (real + virtual): 1632 cores;
- Total memory: 5.3 TeraBytes;
- Disk space for data storage: 85TeraBytes;
- Theoretical peak performance: 19.1 TeraFlops = 19178 GigaFlops
- Interconnection: InfiniBand



- Computational nodes: 36
- Total numbers of cores: 284 cores;
- Total memory: 406 GigaBytes
- Disk space for data storage: 12.4TeraBytes;
- Interconnection: Gigabit Ethernet

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Objetivos

Desenvolvimento de uma ferramenta computacional capaz de simular escoamentos complexos presentes na indústria petrolífera. Exemplos:

- Escoamentos monofásicos;
- Escoamentos bifásicos/multifásicos;
- Escoamentos reativos;
- Escoamentos com a presença de geometrias complexas;
- Escoamentos à variados números de Reynolds;
- Interação fluido-estrutura.



Physical flows aspects that must be modeled

- Shape interfaces;
- Deformable mobile interfaces;
- opposite properties with high aspect ratio;
- Detachment and replacement drops/droplets;
- **9** Bubbles/drops \ll domain \Rightarrow located refinement;
- High Reynolds number \Rightarrow turbulence modeling;
- Surface tension and physical properties \Rightarrow discontinuities;
- Triple contact presence: solid, liquid and gas;
- Physical mechanisms of objects transports and formation (drops, solid particles) and high number and different scales of time and length.

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AMR3d code features

Adaptive Mesh Refinement - AMR3d

- Based on local structured adaptive mesh refinement in space and time;
- Paralle, with MPI domain partition;
- Second order in space and time;
- Temporal discretization: semi-implicit (two phases flow) and implicit (reactives);
- Spatial discretization: finite difference (two phases flow) and finite volumes (reactives);
- Linear Systems: Multigrid-multilvel method, Strong Implicit Procedure (SIP), PETSC;



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AMR3d code features

Adaptive Mesh Refinement - AMR3d

- Volume-of-Fluid Method and e Front-Tracking Method to represent the fluid-fluid interface;
- Immersed Boundary Method to represent the static and rigid budies;
- LES methodology to the turbulence modeling;
- Euler-Lagrange modeling to droplets transport;
- Triple contact line modeling.



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Development historical code



Mathematical Modeling

Governement Equation

 $\rho(\phi)[\mathbf{u}_{\mathsf{t}} + (\mathbf{u} \cdot \nabla)\mathbf{u}] = \nabla \cdot [\mu(\phi)(\nabla \mathbf{u} + \nabla \mathbf{u}^{\dagger})] - \nabla \mathbf{p} + \rho(\phi)\mathbf{g} + \mathbf{f}_{\sigma} + \mathbf{f}_{s},$

 $\nabla \cdot \mathbf{u} = 0.$

 $\rho(\phi) = \rho_c + (\rho_d - \rho_c) \phi(\mathbf{X}, t)$ $\mu(\phi) = \mu_c + (\mu_d - \mu_c) \phi(\mathbf{X}, t)$

\$\phi\$: indicator function
F-T method: level set with sign
VoF method: color function

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Temporal discretization

MEX Schemes	
$\frac{\rho(\phi)^{n+1}}{\Delta t}(\alpha_2)$	$\mathbf{u}^{n+1} + \alpha_1 \mathbf{u}^n + \alpha_0 \mathbf{u}^{n-1}) = \beta_1 f(\mathbf{u}^n) + \beta_0 f(\mathbf{u}^{n-1}) + \beta_0 $
	$\lambda \Big[\theta_2 \nabla^2 \mathbf{u}^{n+1} + \theta_1 \nabla^2 \mathbf{u}^n + \theta_0 \nabla^2 \mathbf{u}^{n-1} \Big] - \nabla \rho^n + \rho^{n+1}(\phi) \mathbf{g},$
	$f(\mathbf{u}) = -\lambda \nabla^2 \mathbf{u} + \nabla \cdot \left[\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) - \mathbf{u} \cdot \nabla \mathbf{u} + \mathbf{f}_{\sigma} \right]$
	$\Delta t_0 + 2\gamma\Delta t_c$ Δt_c
	$\alpha_2 = \frac{\Delta t_0 + 2\gamma \Delta t_1}{\Delta t_0 + \Delta t_1}, \theta_2 = \gamma + c \frac{\Delta t_1}{\Delta t_0 + \Delta t_1}$
	$\alpha_1 = \frac{\Delta t_1 - \Delta t_0 - 2\gamma \Delta t_1}{\Delta t_0}, \ \theta_1 = 1 - \gamma - c \frac{\Delta t_1}{\Delta t_0}$
	$lpha_0=-lpha_1-lpha_2, \ \ heta_0=c\Big(rac{\Delta t_1}{\Delta t_0}-rac{\Delta t_1}{\Delta t_0+\Delta t_1}\Big),$
	$\beta_1 = \frac{\Delta t_0 + \gamma \Delta t_1}{\Delta t}, \ \ \beta_0 = -\gamma \frac{\Delta t_1}{\Delta t},$

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Temporal discretization

IMEX Schemes

- SBDF (Semi Backward Difference Formula): $(\gamma, c) = (1,0)$;
- CNAB (Crack-Nicolson Adans-Bashforth): $(\gamma, c) = (\frac{1}{2}, 0);$
- MCNAB (Modified Crack-Nicolson Adans-Bashforth): $(\gamma, c) = (\frac{1}{2}, \frac{1}{8});$
- CNLF (Cranck-Nicolson Leap-Frog): $(\gamma, c) = (0, 1)$.



Spatial discretization



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Mathematical Modeling



Numerical Methodology



Numerical Methodology



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Adaptive mesh refinement



Adaptive mesh refinement



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Ghosts cells on an adaptive mesh refinement

- Extrapolation on the same level $(* \rightarrow \triangle)$;
- Interpolation on the coarse level, *I* − 1 (● → □);
- Interpolation between *I* and *I* − 1, (△ and □ → ○)
- Importing ghosts cells from simbling grid;
- Apply the real boundary condition.



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Multigrid-Multilevel Algorithm

1:	for $l = l_{top} a 1$ do	
2:	if $l = l_{top}$ then	
3:	$e^{l_{ltop}}=0$	
4:	Calcule $L(\overline{\phi})$, em $\Omega^{l_{top}}$	
5:	$R^{l_{top}} \leftarrow B^{l_{top}} - L(\overline{\phi})^{l_{top}}$ e	$m \Omega^{I_{top}}$
6:	$e^{l_{ltop}} \leftarrow RBGS(A^{l_{ltop}}, e^{l_{ltop}})$	$(P^{p}, R^{l_{ltop}}) \operatorname{em} \Omega^{l_{top}}$
7:	else	
8:	$e_l = 0$	
9:	Calcule $L(\overline{\phi})^{I}$, em Ω^{I}	
10:	Calcule $L(e)^{\prime}$, em $\delta \Omega^{\prime+}$	-1
11:	$R' \leftarrow B' - L(\overline{\phi})'$, em Ω'	$1 - \Omega^{l+1}$
12:	$R' \leftarrow \mathscr{R}_{l}^{l+1}(R' - L(e'))$, em $P(\Omega_l^{l+1})$
13:	$e' \leftarrow RBGS(A', e', R')$	$\operatorname{em} \Omega'$
14:	end if	
15:	end for	< □ > < 图 > < 差 > < 差 > 差 の < @
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Interface Modeling

Method	Pros	Cons	
Loval Sat	Conceptually simple	Limited precision	
Level Set	Easy implementation	Non conservative	
Charle Contura	Easy implementation	Numerical diffusion	
Shock Capture	Multiple advective Schemes available	Requires fine meshes	
	Extremely accurate	High computational cost	
Marker Particle	Robust	Marker particles must be	
	Can handle great topological changes	redistributed	
	Conceptually simple	Numeric diffusion	
SLIC VOF	Easy extension to 3D	Limited precision	
		Artificial fragmentation and	
		coalescence	
	Relatively simple	Artificial fragmentation and	
PLIC VOF	Precise	coalescence	
	Supports great topological changes		
Lattice Deltromon	Precise	Difficult to implement	
Lattice Boitzammi	Supports great topological changes	Artificial fragmentation and	
		coalescence	
	Extremely Precise	Requires mapping	
Front Trocking	Robust	Requires dynamic remeshing	
FIGHT HACKING	Supports great topological changes		
	No artificial coalescence or fragmentation (D) (P) (P) (P) (P)		

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Curvat	ure
۲	Parabolic fitting: fit a curve, or mathematical function, that has the best fit to a series of data points. Fit a parabola (paraboloid in 3D) by minimising $F(a_i) \equiv \sum_{1 \le j \le n} [z'_j - f(a_i, x'_j)]$ with $f(a_i, x)] \equiv a_0 x^2 + a_1 y^2 + a_2 xy + a_3 X + a_4 y + a_5$ $\kappa \equiv 2 \frac{a_0(1+a_4^2)+a_1(1+a_3^2)-a_2a_3a_4}{(1+a_3^2+a_4^2)^{3/2}}$
•	Least Square: based on a least-squares fit of a Taylor series to determine the derivatives of the colour function field and the derivatives of the interface normal vector. Taylor series is developed for the colour function field around cell P with its neighbours Q: $\gamma_Q \equiv \gamma_P + \frac{\partial \gamma}{\partial x_i} _p(x_{i,Q} - x_{i,P}) + \frac{\partial^2 \gamma}{\partial x_i \partial x_j} _p(x_{i,Q} - x_{i,P})(x_{j,Q} - x_{j,P}) + O(\Delta x_i^3)$ $A \cdot \phi = b$ $\kappa = -\frac{\partial m_i}{\partial x_i} _p$

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Equations

$$\begin{aligned} \delta F_{\sigma} &= \oint_{\delta \Gamma} \sigma \mathbf{t} \times \mathbf{n} d\Gamma, \\ \mathbf{f}_{\sigma}(\mathbf{x}, t) &= \int \mathbf{F}_{\sigma}(\mathbf{X}, t) D(\mathbf{X} - \mathbf{x}) d\mathbf{X}, \\ \rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u}\right) &= \nabla \cdot \left(\mu(\nabla \mathbf{u} + \nabla \mathbf{u}^{T})\right) - \nabla \rho + \rho \mathbf{g} + \mathbf{f}_{\sigma}, \\ \nabla \cdot \mathbf{u} &= 0, \\ \mathbf{U}(\mathbf{X}, t) &= \int \mathbf{u}(\mathbf{x}, t) D(\mathbf{x} - \mathbf{X}) d\mathbf{x} \\ \frac{\partial \mathbf{X}(t)}{\partial t} &= \mathbf{U}(\mathbf{X}(t), t). \end{aligned}$$

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	$D(\mathbf{x} - \mathbf{X}) = \frac{1}{h_x h_y h_z} W\left(\frac{x - X}{h_x}\right) W\left(\frac{y - Y}{h_y}\right) W\left(\frac{z - Z}{h_z}\right),$	
here	$W(r) = \begin{cases} \frac{1}{4}(1 + \cos(\frac{\pi}{2}r)), & r < 2, \\ 0, & r \ge 2, \end{cases}$	
nd	$r=\frac{x-X}{h_x},\frac{y-Y}{h_y},\frac{z-Z}{h_z}.$	
	$egin{aligned} \mathcal{H}(arphi) = \left\{ egin{aligned} 1, & arphi > \gamma \ 0.5(1+rac{arphi}{\gamma}+rac{1}{\pi}sin(rac{\piarphi}{\gamma})), & \ arphi\ \leq \gamma \ 0, & arphi < -\gamma \end{aligned} ight. \end{aligned}$	
	$\Psi(\varphi) = H(\varphi)\Psi_1 + (1 - H(\varphi))\Psi_2$	

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Lagrangian Interface

GTS - GNU Triangulated Library

- Conservative Remeshing based on edge collapse.
 - Memoryless Polygon Simplification, Lindstrom and Turk (1999)
- Preserves geometry volume, area and shape; element quality



Lagrangian Interface

GTS - GNU Triangulated Library

- Conservative Remeshing based on edge collapse.
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VRA - Volume Recovery Algorithm

• Volume change is small and uniform over the whole surface



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Immersed Boundary











Coeficiente de Arrasto (C_d)						
Re	Referência	Escama	%			
10^{2}	1.8035	1.9448	+7,83			
10^{3}	0.7252	0.7490	+3,28			
10^{4}	0.6467	0.6103	-5,63			
10^{5}	0.6276	0.6052	-3,57			
10^{6}	0.6286	0.6070	-3,44			

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Flow in fans

General data

- Volumetric flow 60 T/h, ou 16 Nm³/s with rotation of 1650 RPM;
- Work temperature 69.2 °C;
- Density: $\rho = 0.5842 \, kg/m^3$;
- Viscosity: 8.659×10^{-6} Pa.s;
- Maximum reynolds number, based in the inlet boundary condition ≈ 2.2 milhões;
- Maximum reynolds number, based in rotor speed ≈ 36.85 milhões;



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Flow in fans



Fluid structure interaction example



Numerical features that are in progress

- Flow with high physical ratio;
- Solvers with best speedup;
- Isothermic flows;
- Contact triple modeling in complex geometries;
- Euler-lagrange modeling to droplets transport;
- Flows in presence of mobile complex geometries;
- Turbulence Modeling;
- Graphic interface.



Acknowledgements

