ADVANCED COMPUTING

UTAustin Portugal

HPC method for steady state 2D convection-diffusion equation on complex geometries

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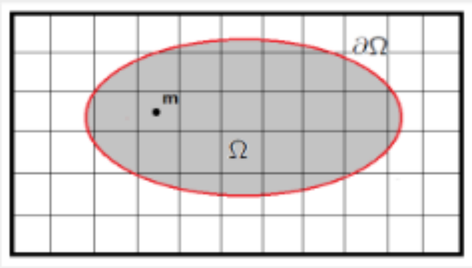
Background

High Performance Computing is efficient when the algorithms take advantage of the hardware and computer architecture. Well structured data combined with independent routines can lead to optimal parallelization and performance scaling. Consequently, finite volume or difference on Cartesian grid is still the best choice for numerical simulation of physical processes. The most popular methods involve unstructured meshes due to the geometry constraints but we propose a new method that uses structured meshes.

- Domain Ω is an open connected set with a **curved** boundary ∂Ω (Jordan curve).
- **Very high** accurate solution for equation:
$$-\nabla.(L\nabla\phi)+\nabla.(U\nabla\phi)=f(x,y)\text{ in }\Omega$$
with complex geometries that do not fit the grid.

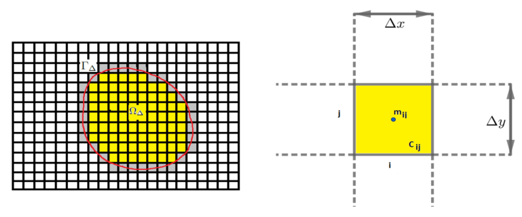


- General Robin boundary conditions (bc),
$$\beta\phi(P)+\gamma\nabla_x\phi(P).\vec{n}=g(P)$$

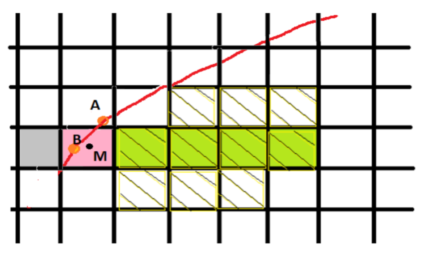
Methodology

Real domain Ω is substituted by the computational domain Ω_Δ composed of grid cells (fig. **a** - yellow) surrounded with ghost cells (fig. **a** - grey). ROD technique is used to approximate solution ϕ at the centroid M, using 2 points of the collar (fig. **b** - A, B) and data associated to a stencil (fig. **b** - dashed cells).
Alternate Direction Implicit (infogram **c**) splits the 2D problem into N independent 1D problems. This is highly parallelizable and provides an efficient way to perform computation with many-cores.

a)



b)



Using differential operators,
$$G_x=-L\frac{\partial^2}{\partial x^2}+U\frac{\partial}{\partial x};G_y=-L\frac{\partial^2}{\partial y^2}+\frac{\partial}{\partial y}$$
one obtains the CD eq:
$$(G_x+G_y)\phi=f$$
Using 2nd or 4th-order centered FD approx.,
$$G_{\Delta x}\phi_{i,j}=-\frac{L}{\Delta x^2}[\phi_{i+1,j}-2\phi_{i,j}+\phi_{i-1,j}]+\frac{U}{2\Delta x}[\phi_{i+1,j}-\phi_{i-1,j}]$$
Lead to discretized CD eq.,
$$(G_{\Delta x}+G_{\Delta y})\phi_\Delta=f_\Delta$$
Using **ADI** one solves lines/columns at each half step as,
$$(\alpha I+G_{\Delta x})\phi_\Delta^{n+1/2}=(\alpha I-G_{\Delta y})\phi_\Delta^n+f_\Delta\,(lines)$$
$$(\alpha I+G_{\Delta y})\phi_\Delta^{n+1}=(\alpha I-G_{\Delta x})\phi_\Delta^{n+1/2}+f_\Delta\,(columns)$$

c)

Results

We considered a grid]0,2[x]0,2[with NxN cells with the physical domain $(x-1)^2+(y-1)^2\leq 0.5^2$ and exact solution $\phi(x,y)=exp(x+2y)$
We performed tests using 2 Xeon E5-2650v2 2.6GHz, 20MB L3 and 16 cores (UMinho, DI, SEARCH Cluster).
Table **a** shows the results of solving the problem with ADI for different grid sizes while table **b** shows the scaling/speed up using a parallel code.

nx	its	time	time/it
80	144	0.03	2.04E-4
160	250	0.18	7.20E-4
320	430	1.27	29.5E-4
640	803	8.27	103E-4
1280	1652	83.69	506E-4
2560	3649	679	1860E-4

a)

grid: 2560 x 2560

Cores	Time (s)	Speed up
1	679	x
2	376	1.81
4	226	3.00
8	138	5.22
16	78	8.71

b)

Impact/Conclusions

We developed a first class of numerical methods based on the ADI coupling with the ROD method to provide very high order approximations for the 2D convection diffusion problem. We obtain very good speed-up while the optimal order is preserved. We expect to briefly adapt the technique to the Navier-Stokes equations and demonstrate the efficiency of the method. Applications in aeronautics (plane), aeroespacial (aircraft), and energy (heat transfer) are the main opportunities in future developments.

- Inverse paradigm: think the numerical scheme in function of the hardware, not the contrary.
- ROD technology enables structured grid even with complex geometrie and provide efficient hardware usage
- Good overall performance with potential to improve the scalability.

UTAustin Portugal FCT Fundação para a Ciência e a Tecnologia TEXAS The University of Texas at Austin CENTROALGORITMI CF-UM-UP NORTE2020 Lisb@20[20] COMPETE 2020 CENTRO 2020