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Developing Highly Scalable Fluid Solvers for Enabling Multiphysics Simulation

LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Early Career R&D Program

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Problem

Computing hardware is trending towards distributed, massively parallel architectures in order to achieve high computational throughput. For example, Cielo uses 43,104 cores, Intrepid at Argonne uses 163,840 cores, and the new ASC machine Sequoia at Lawrence Livermore uses 1.6 million cores. This proposal seeks to develop a fluid simulation algorithm based on artificial compressibility (AC) that is capable of scaling on these and future systems.

Approach

Traditional incompressible-flow solvers are based on the incompressible Navier--Stokes (NS) equations, in which the continuity equation acts as a constraint imposing a divergence-free velocity field. In this case, no direct coupling of pressure to velocity exists requiring an implicit solution.

Explicit fluid simulation algorithms necessarily imply artificial compressibility (AC), which allows for a local update procedure resulting in excellent scalability on order 100,000 processors. However, as originally formulated, the AC method shows transient errors that must be addressed. The proposed solution uses a reformulation of the NS equations to eliminate these errors while retaining an explicit formulation.

Standard AC

continuity + *thermo. rel.* = *pressure evolution*

isentropic assumption

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{u} \quad + \quad \mathrm{d}\rho = \mathrm{Ma}^2\mathrm{d}P - B\left(\frac{\mathrm{Pr}\gamma\mathrm{Ma}^2}{A}T + 1\right)\mathrm{d}s \;(\to 0) \quad = \quad \frac{\partial P}{\partial t} \approx -\frac{1}{\mathrm{Ma}^2}\nabla\cdot\boldsymbol{u}$$

Entropically Damped AC (EDAC)

continuity + *alt. thermo. rel.* + *entropy bal.* = *pressure evolution*

alternate thermo. rel.

$$\mathrm{d}P \approx \frac{\mathrm{Pr}B}{A}\mathrm{d}T$$

$$\frac{\mathrm{d}\rho}{\rho} = \gamma\mathrm{Ma}^2\left(\mathrm{d}P - \frac{\mathrm{Pr}B}{A}\mathrm{d}T\right) \to 0$$

EDAC pressure evolution

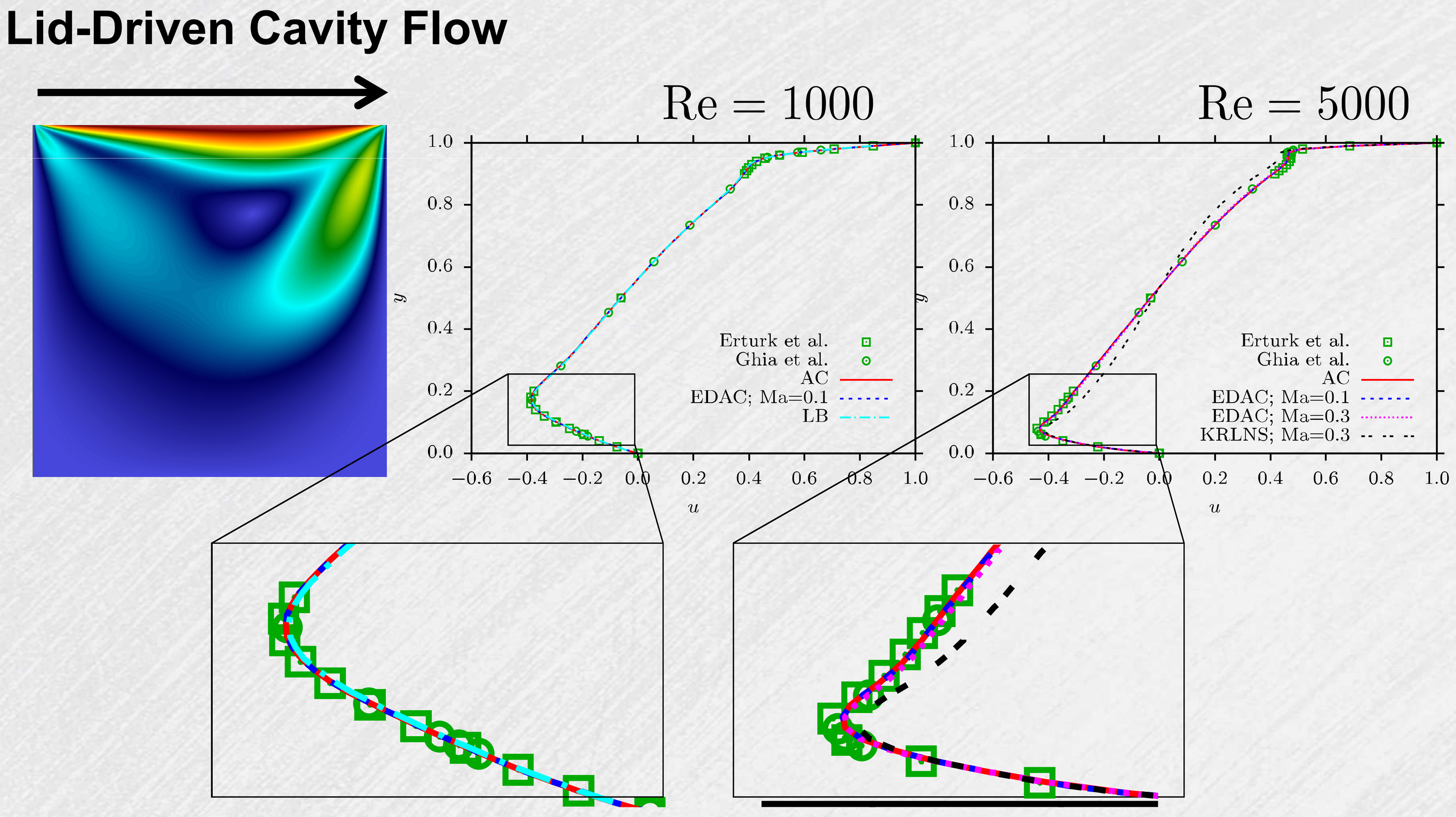
$$\frac{\mathrm{D}P}{\mathrm{D}t} = -\frac{1}{\mathrm{Ma}^2}\nabla\cdot\boldsymbol{u} + \frac{1}{\mathrm{Re}}\nabla^2 P$$

nomenclature

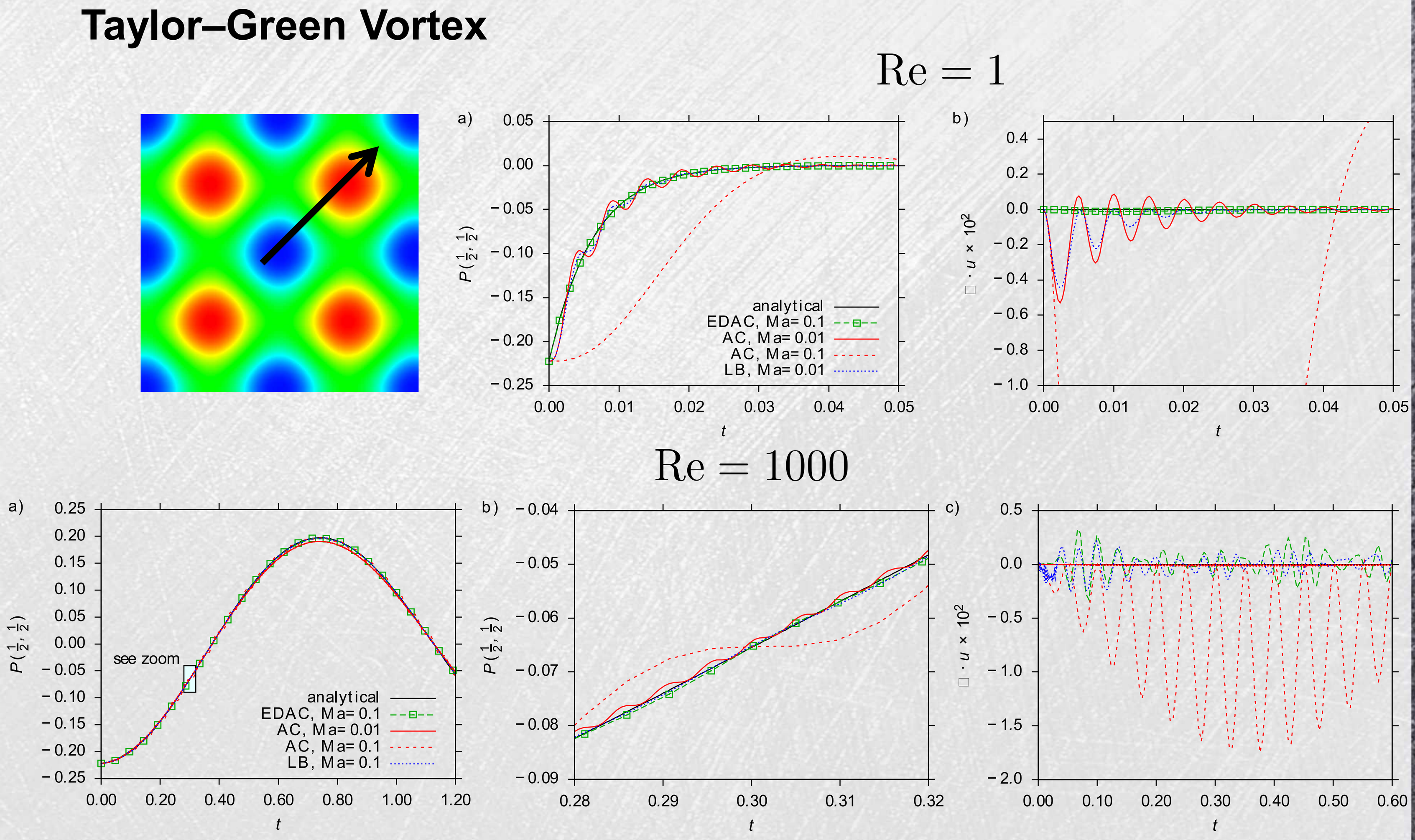
- Ma Mach number
- Re Reynolds number
- Pr Prandtl number
- T temperature
- Φ viscous dissipation
- s entropy
- ρ density
- $\boldsymbol{u}$ velocity
- P pressure
- $\boldsymbol{\tau}$ viscous stress
- γ ratio spec. heats
- $A \equiv \rho\alpha c_p T_0$
- $B \equiv \beta T_0$

Results

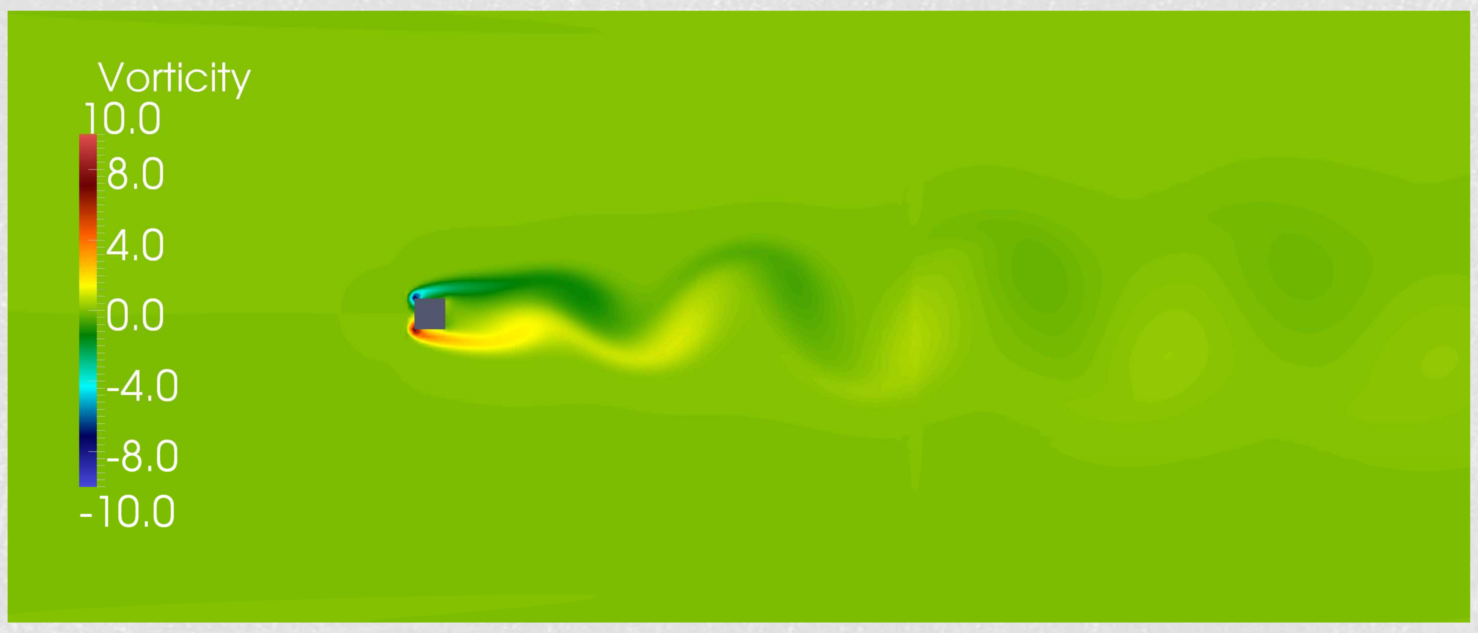
Lid-Driven Cavity Flow



Taylor–Green Vortex



Vortex Shedding



Significance

Advanced fluid simulation capabilities are integral to maintaining the viability and safety of the nuclear weapons stockpile. Highly scalable methods, such as the method proposed here, are required to leverage the increasingly parallel computational platforms used by Sandia National Laboratories and the NNSA in pursuit of this mission.

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