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Fully Explicit Algorithms for Fluid Simulation

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Thermal and Fluid Processes, Sandia National Laboratories

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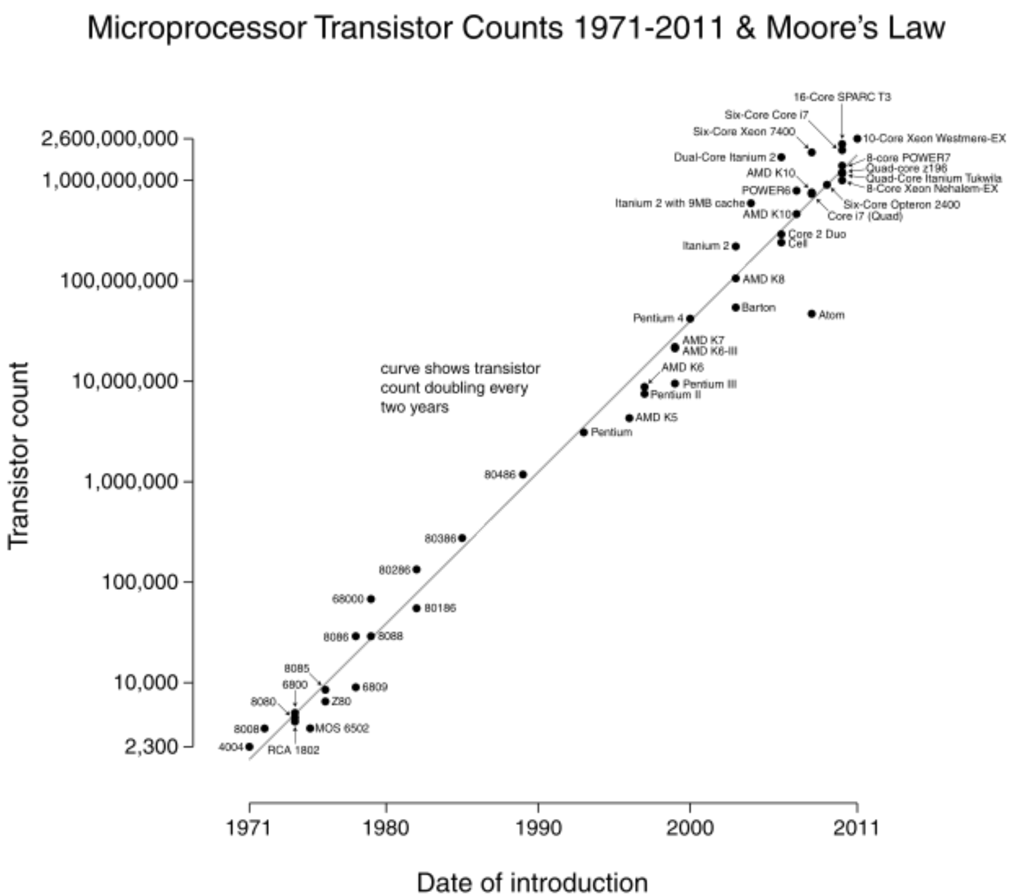
Motivation



Today, Moore's law implies increasing parallelism

LLNL Sequoia ~ 1.6 million cores

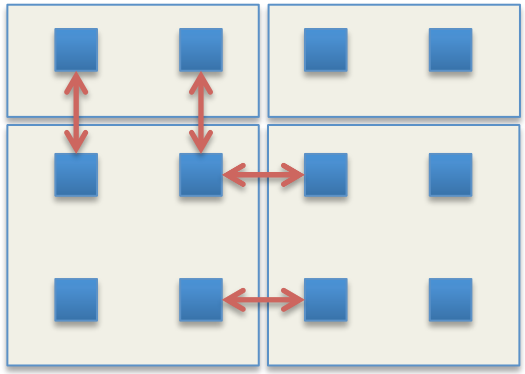
source: wikipedia.org

Pseudo-compressible Methods

Artificial Compressibility (AC)

Chorin (1967) $$P = \frac{1}{\mathrm{Ma}^2}\rho$$

local information propagation



Kinetically Reduced Local Navier–Stokes (KRLNS)

Ansumali, Karlin, and Ottinger (2005)
Karlin, et al. (2006)
Borok, Ansumali, and Karlin (2007)

$$\frac{\partial G}{\partial t} = -\frac{1}{\mathrm{Ma}^2} + \frac{1}{\mathrm{Re}}\nabla^2 G \qquad G = P - \frac{u^2}{2}$$

Lattice-Boltzmann Method (LBM)

$$P = c_s^2\rho$$

Entropically Damped Artificial Compressibility (EDAC)

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Compressible Navier–Stokes

$$\frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{u}$$

cons. mass

$$\rho\frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = -\nabla P + \frac{1}{\mathrm{Re}}\nabla\cdot\boldsymbol{\tau}$$

cons. mom.

$$\left(\frac{\mathrm{Pr}\gamma\mathrm{Ma}^2}{A}T+1\right)\frac{\mathrm{D}s}{\mathrm{D}t} = \frac{\mathrm{Ma}^2\gamma}{A}\frac{1}{\mathrm{Re}}\left(\nabla^2 T+\Phi\right)$$

cons. entropy
(energy)

$$f(P,\boldsymbol{u},s)$$

$$\mathrm{d}\rho = \mathrm{Ma}^2\mathrm{d}P - B\left(\frac{\mathrm{Pr}\gamma\mathrm{Ma}^2}{A}T+1\right)\mathrm{d}s$$

$$T = T(P,s)$$

thermo. state

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

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Standard AC

to eliminate equation, we must constrain variable!

$$\mathrm{d}s = 0$$

isentropic sound propagation

$$\underbrace{\cancel{\mathrm{d}\rho = \mathrm{Ma}^2 \mathrm{d}P - B\left(\frac{\mathrm{Pr}\,\gamma\,\mathrm{Ma}^2}{A} T + 1\right)\mathrm{d}s} \qquad \frac{1}{\rho}\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\nabla\cdot\boldsymbol{u}}$$

$$\frac{\mathrm{D}P}{\mathrm{D}t} = -\frac{1}{\mathrm{Ma}^2}\nabla\cdot\boldsymbol{u} \qquad \rho = 1 + O(\mathrm{Ma}^2)$$

$$\frac{\partial P}{\partial t} \approx -\frac{1}{\mathrm{Ma}^2}\nabla\cdot\boldsymbol{u}$$

implications of no entropy production

EDAC

selection of $\mathrm{d}s = 0$ **is arbitrary**

$$\frac{\mathrm{D}\rho}{\mathrm{D}t} = -\rho\nabla\cdot\boldsymbol{u} = \mathrm{Ma}^2\frac{\mathrm{D}P}{\mathrm{D}t} \underbrace{- \frac{B}{A}\frac{\mathrm{Ma}^2\gamma}{\mathrm{Re}}\left(\nabla^2 T + \Phi\right)}_{\sim\,\mathrm{d}s}$$

continuity + density + energy

alternative thermodynamic constraint

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

$$\mathrm{d}P \approx \frac{\mathrm{Pr}B}{A}\mathrm{d}T \qquad B \equiv \beta T_0$$

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

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

Discretization Method

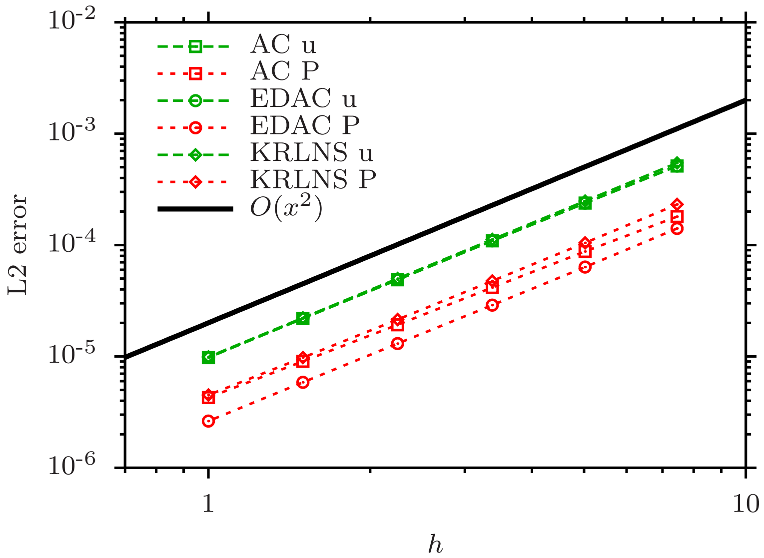
MacCormack finite-difference method (AC, EDAC, KRLNS) $O(\Delta x^2, \Delta t^2)$

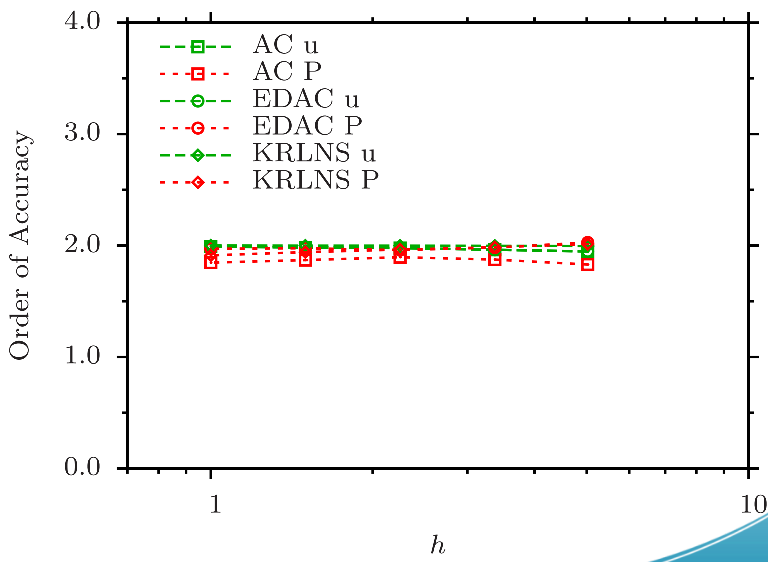
Traveling Wave code verification (MMS to isolate discretization error)

$$u = \frac{1}{3} + \frac{2}{3}\cos\left[2\pi\left(x - \frac{t}{3}\right)\right]\sin\left[2\pi\left(y - \frac{t}{3}\right)\right]\exp\left(\frac{-8\pi^2 t}{\mathrm{Re}}\right)$$

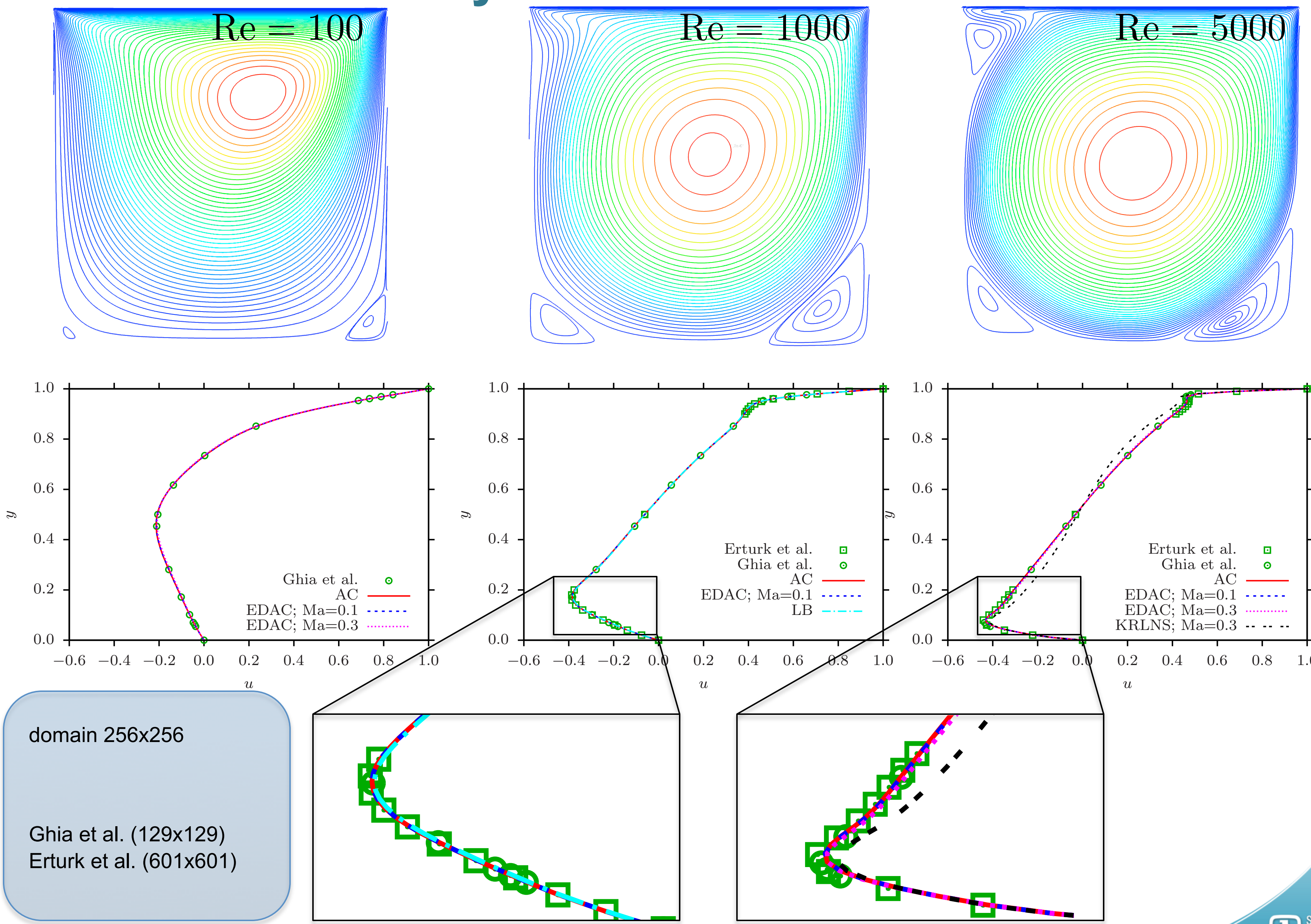
$$v = \frac{1}{3} - \frac{2}{3}\sin\left[2\pi\left(x - \frac{t}{3}\right)\right]\cos\left[2\pi\left(y - \frac{t}{3}\right)\right]\exp\left(\frac{-8\pi^2 t}{\mathrm{Re}}\right)$$

$$P = -\frac{1}{9}\left\{\cos\left[4\pi\left(x - \frac{t}{3}\right)\right] + \cos\left[4\pi\left(y - \frac{t}{3}\right)\right]\right\}\exp\left(\frac{-16\pi^2 t}{\mathrm{Re}}\right)$$





Lid-Driven Cavity Flow



domain 256x256

Ghia et al. (129x129)
Erturk et al. (601x601)

Traveling Taylor–Green Vortex

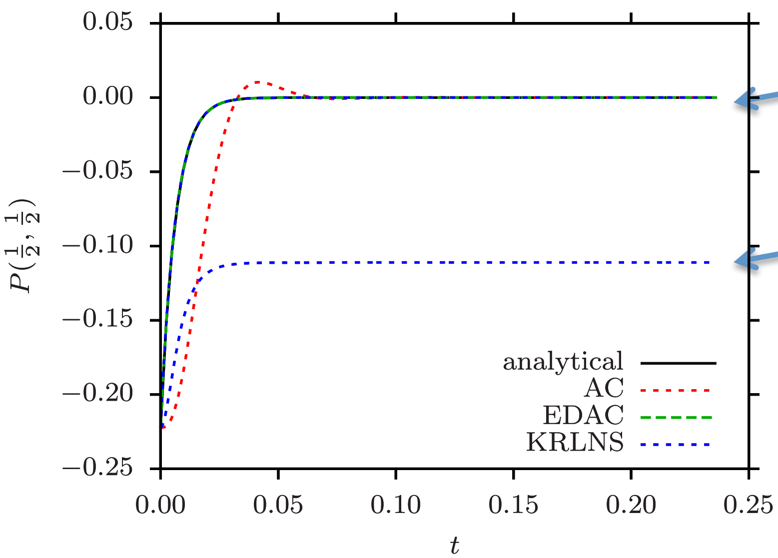
simulation details

65 x 65 domain
Ma = 0.1
Re = 1

analytical solution

$$u = \frac{1}{3} + \frac{2}{3}\cos\left[2\pi\left(x - \frac{t}{3}\right)\right]\sin\left[2\pi\left(y - \frac{t}{3}\right)\right]\exp\left(\frac{-8\pi^2 t}{\mathrm{Re}}\right)$$

$$P = -\frac{1}{9}\left\{\cos\left[4\pi\left(x - \frac{t}{3}\right)\right] + \cos\left[4\pi\left(y - \frac{t}{3}\right)\right]\right\}\exp\left(\frac{-16\pi^2 t}{\mathrm{Re}}\right)$$



added correction term to KRLNS $\dfrac{1}{\mathrm{Re}}\nabla \boldsymbol{u} : \nabla \boldsymbol{u}$

qualitatively incorrect behavior for KRLNS

Traveling Taylor–Green Vortex

simulation details

65 x 65 domain
Ma = 0.1
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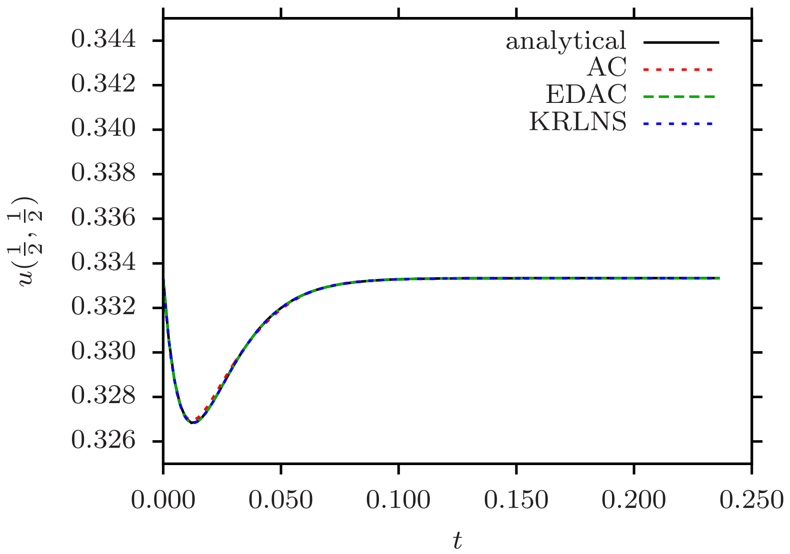
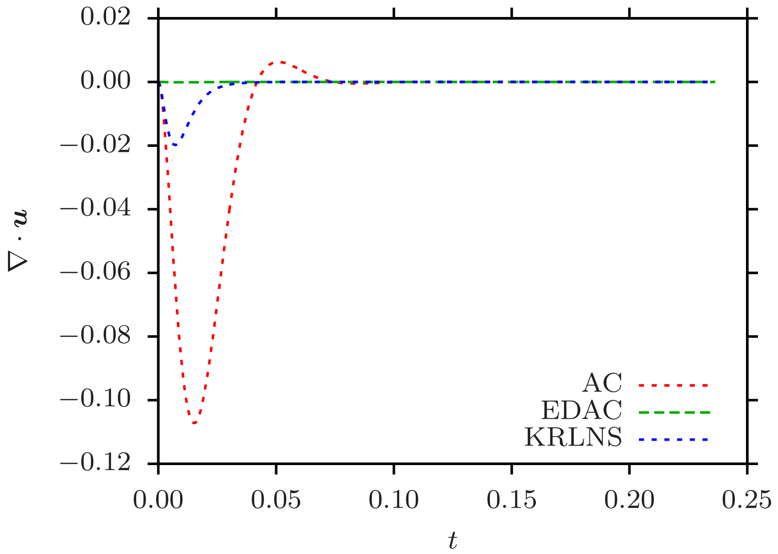
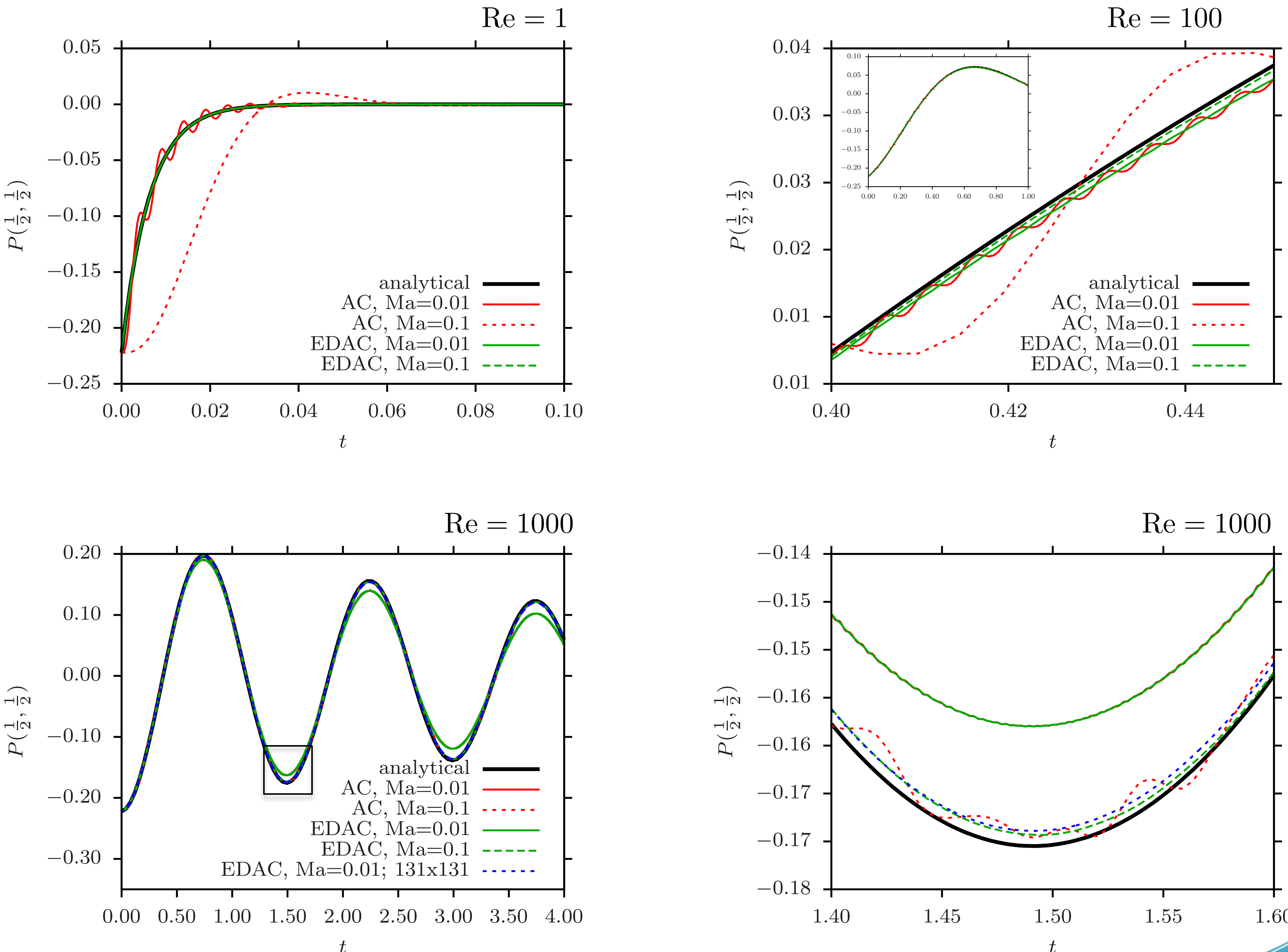
$$\frac{\mathrm{d}\rho}{\rho} = \gamma \mathrm{Ma}^2 \left(\mathrm{d}P - \frac{\mathrm{Pr} B}{A} \mathrm{d}T \right) \to 0$$

recall that EDAC thermodynamic relationship limits density/divergence fluctuations





Traveling Taylor–Green Vortex



Conclusions & Future Work

Traditional AC methods show pressure fluctuations

KRLNS contains error

EDAC method shows time-accurate pressure

particularly at moderate/low Re

Next steps

Performance of EDAC method in dual time stepping methods

Questions?