

On Stabilized Finite Element Methods for Transient Problems with Varying Time Scales

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Petropolis, August 9-13, 2004



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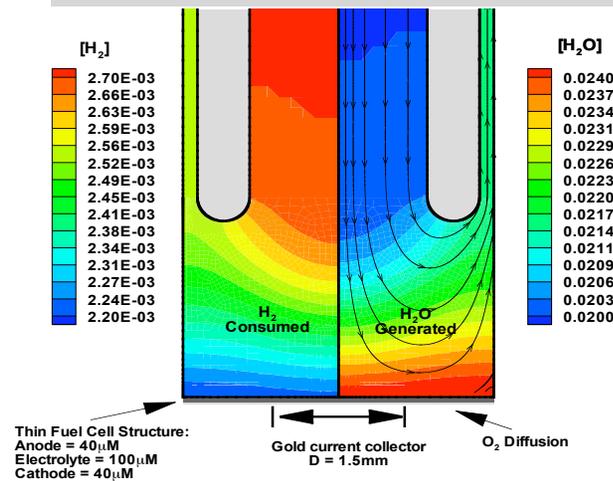


Problems with multiple time scales at Sandia: MP Salsa, CHARON

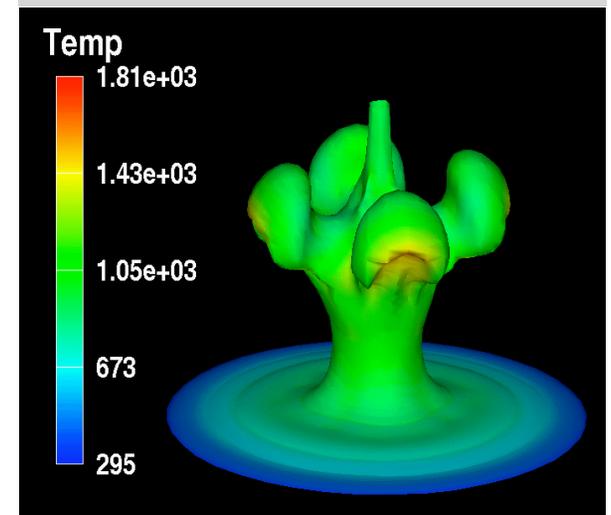
Applications:

- ✓ Catalysis
- ✓ Chemical Detectors
- ✓ Combustion
- ✓ CVD
- ✓ Semiconductors
- ✓ MEMS

Simulation of Experimental Solid Oxide Fuel Cell



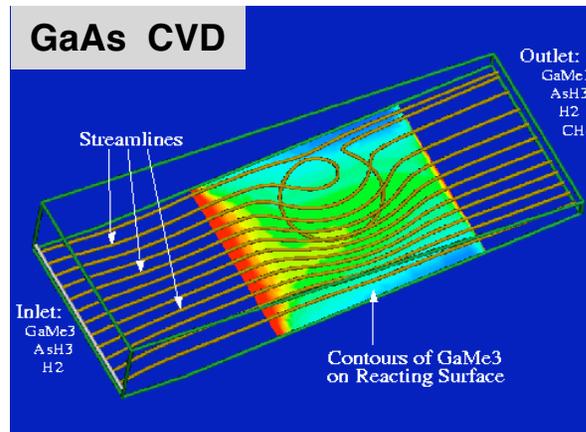
Turbulent Combustion Simulation Of Methanol Pool Fire



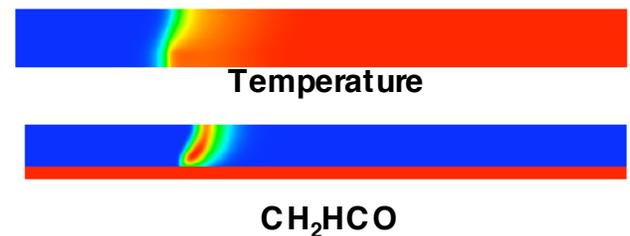
Processes

- Chemical kinetics
- Momentum diffusion
- Heat conduction
- Convection

GaAs CVD



Ethane Catalysis





Model equations and their discretization

PDE Model $\left\{ \begin{array}{l} \rho \dot{\mathbf{u}} - \nabla \cdot \mathbf{T} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p = \rho \mathbf{g} \\ \nabla \cdot (\rho \mathbf{u}) = 0 \end{array} \right\} + \left\{ \begin{array}{l} \text{species fraction} \\ \text{thermal energy} \end{array} \right\}$

Discrete equations

- *Spatial Discretization* = Q1 -Q1 + **inf-sup** & **upwind** stabilization

$$\int_{\Omega} (\rho \dot{\mathbf{u}} - \nabla \cdot \mathbf{T} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p) \cdot \mathbf{v} d\Omega + \int_{\Omega} q \nabla \cdot (\rho \mathbf{u}) d\Omega + \sum_{K \in \Omega_h} \int_K \tau(K) (\rho \dot{\mathbf{u}} - \nabla \cdot \mathbf{T} + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla p) \cdot (\rho \dot{\mathbf{v}} - \nabla \cdot \mathbf{S} + \rho \mathbf{u} \cdot \nabla \mathbf{v} + \nabla q) d\Omega + (\text{other equations}) = \int_{\Omega} \rho \mathbf{g} \cdot \mathbf{v} d\Omega \quad \forall (\mathbf{v}, q) \in \mathbf{V} \times S$$

- *Stabilization parameter:* $\tau = \left[\left(\frac{2\rho}{\Delta t} \right)^2 + \rho^2 u_i g_{ij} u_j + 9(2\mu)^2 \frac{g_{ij} g_{ij}}{3} \right]^{-1/2}$
- *Temporal Discretization* = generalized α -method

Computational issues

Time scales

- Chemical kinetics: 10^{-12} to 10^{-5}
- Momentum diffusion: 10^{-6}
- Heat conduction: 10^{-6}
- Convection: 10^{-3} to 10^{-1}



Scales not well-separated!

Time integration issues

- Application of *operator-split* methods accompanied by *instabilities* due to the complex multiphysics (Shadid, Ropp, Ober, JCP 2004)
- *Fully implicit* solvers and *physics based* preconditioners preferred for *stability* and stiff diffusion terms
- Resolving non-equilibrium chemical reaction requires *time steps* orders of magnitude *smaller* than those normally required for the *flow solver*
- Pressure *instabilities* and loss of *convergence* observed for $\Delta t \ll 1$

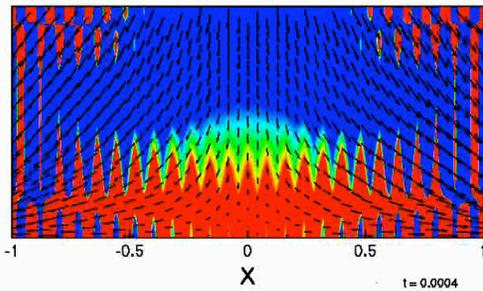


C. Ober, J. Shadid, unpublished

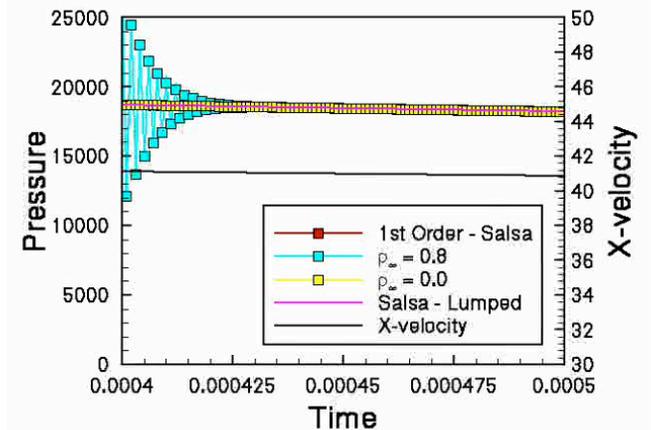
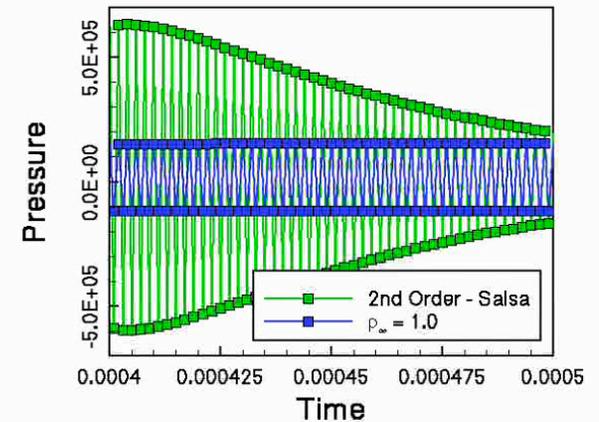
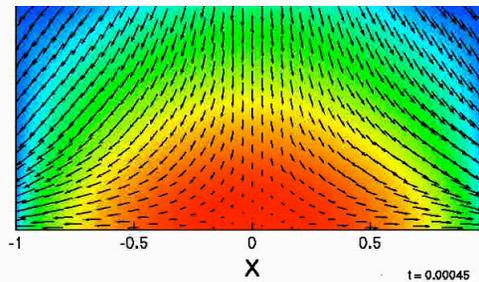
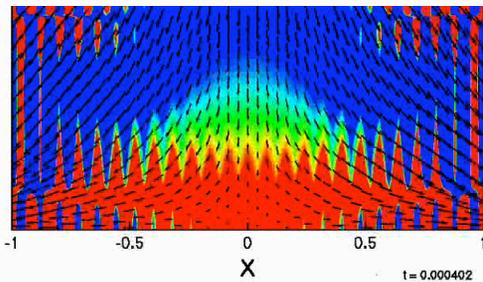
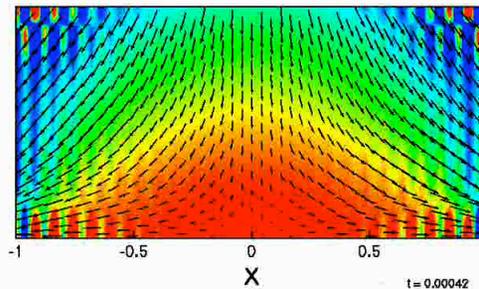
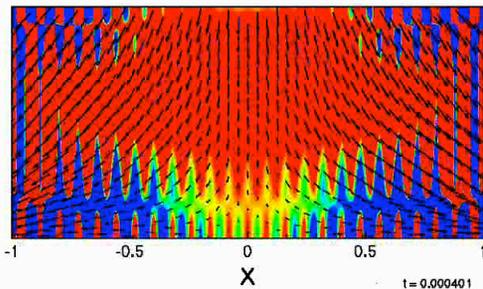
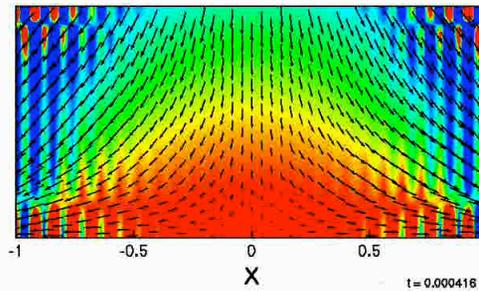
Pressure instabilities: MP Salsa

Pressure instability: was removed by using high wave number damping in time integration (generalized – alpha method); short spurious transient remained

Stagnation Point - 2nd order ($\rho_\infty=0.8$)



Stagnation Point - 2nd order ($\rho_\infty=0.8$)

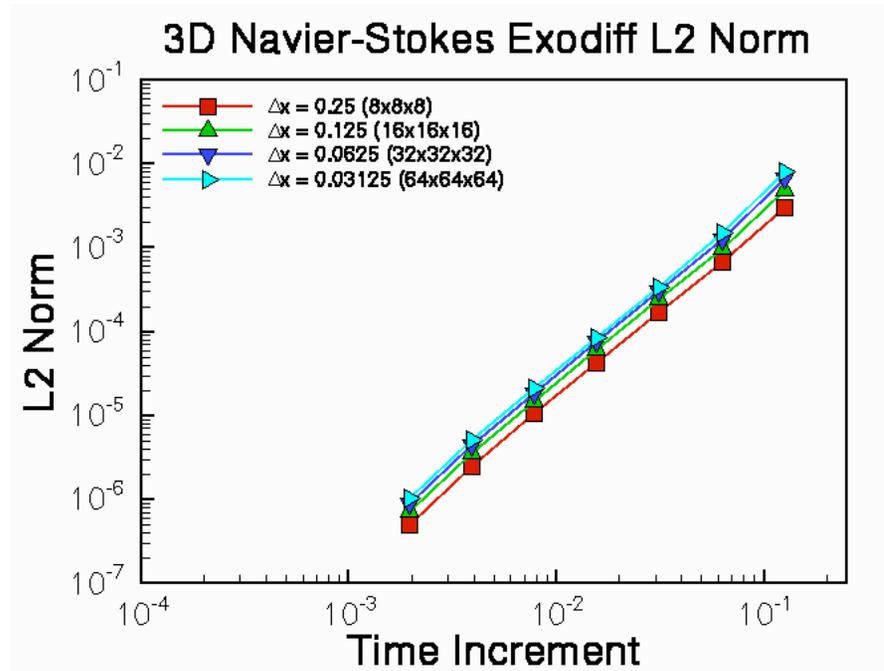
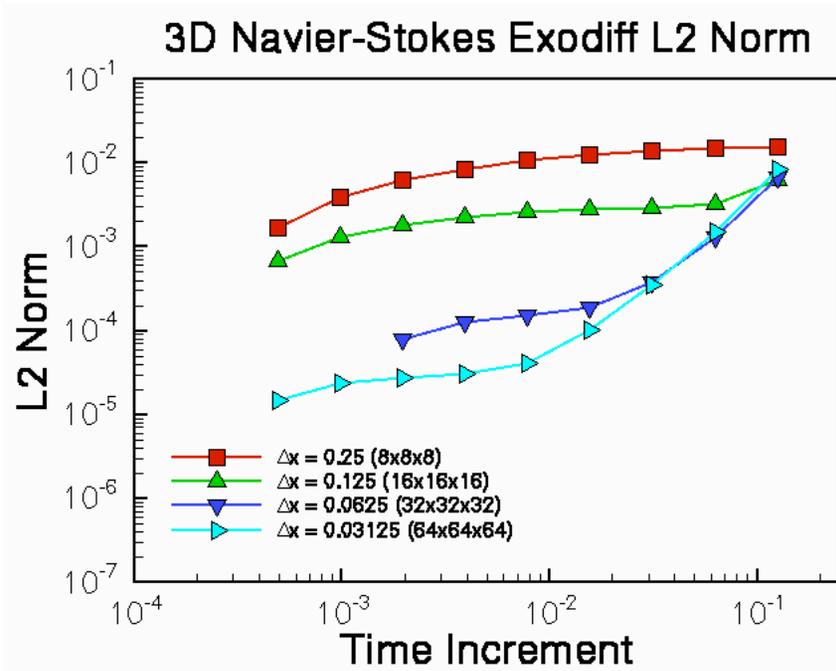


Convergence stagnation

Analytic 3D Navier-Stokes Solution

Δt included in τ

Δt removed from τ



Modification of τ helped to offset stagnation.

Observations relevant to our study

- Size of Δt governed by *reaction rates*, not *accuracy*
- Problems encountered are *not due* directly to *reaction terms*
- *Pressure* rather than *velocity* instabilities indicate that the nonlinear *advective* terms are *not the cause* of the problem
- Convergence stagnation is due to the *limiting* behavior of τ .

$$\tau_m = \left[\left(\frac{2\rho}{\Delta t} \right)^2 + \rho^2 u_i g_{ij} u_j + 9(2\mu)^2 \frac{g_{ij} g_{ij}}{3} \right]^{-1/2} \xrightarrow{\Delta t \rightarrow 0} O(\Delta t)$$

Conjecture: combination of **inf-sup stabilization**, designed to relax a spatial constraint, with **implicit** time integration causes **problems at small time steps**

It suffices to consider the time-dependent Stokes problem with $\tau = \delta h^2$, θ -method



Stabilized Stokes formulations

Spatially stabilized semi-discrete equation

$$\left\{ \begin{array}{c} (\dot{\mathbf{u}}_h, \mathbf{v}_h) \\ - \sum_K \tau_K \int_K \dot{\mathbf{u}}_h \cdot w(\mathbf{v}_h, q_h) dx \end{array} \right\} + \left\{ \begin{array}{c} a(\mathbf{u}_h, \mathbf{v}_h) - b(p_h, \mathbf{v}_h) - b(q_h, \mathbf{u}_h) \\ - \sum_K \tau_K \int_K (-\Delta \mathbf{u}_h + \nabla p_h - \mathbf{f}) \cdot w(\mathbf{v}_h, q_h) dx \end{array} \right\} = (\mathbf{f}, \mathbf{v}_h)$$

Fulfill consistency

$$w(\mathbf{v}_h, q_h) = \begin{cases} \nabla q_h & \text{SGLS} \\ -\Delta \mathbf{v}_h + \nabla q_h & \text{GLS} \\ \Delta \mathbf{v}_h + \nabla q_h & \text{RGLS} \end{cases}$$

Fully discrete equation: θ -method

$$\left\{ \begin{array}{c} (\mathbf{u}_h^{k+1}, \mathbf{v}_h) \\ - \sum_K \tau_K \int_K \mathbf{u}_h^{k+1} \cdot w(\mathbf{v}_h, q_h) dx \end{array} \right\} + \Delta t \left\{ \begin{array}{c} a(\mathbf{u}_h^\theta, \mathbf{v}_h) - b(p_h^\theta, \mathbf{v}_h) - b(q_h, \mathbf{u}_h^\theta) \\ - \sum_K \tau_K \int_K (-\Delta \mathbf{u}_h^\theta + \nabla p_h^\theta - \mathbf{f}^\theta) \cdot w(\mathbf{v}_h, q_h) dx \end{array} \right\} = (\mathbf{f}_h^\theta, \mathbf{v}_h)$$

$$X^\theta = (1 - \theta)X^k + \theta X^{k+1}$$



Stability analysis of one implicit step

Bilinear form

$$Q(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h) = \left\{ \begin{array}{l} (\mathbf{u}_h, \mathbf{v}_h) \\ - \sum_K \tau_K \int_K \mathbf{u}_h \cdot \mathbf{w}(\mathbf{v}_h, q_h) dx \end{array} \right\} + \Delta t \left\{ \begin{array}{l} a(\mathbf{u}_h^\theta, \mathbf{v}_h) - b(p_h^\theta, \mathbf{v}_h) - b(q_h, \mathbf{u}_h^\theta) \\ - \sum_K \tau_K \int_K (-\Delta \mathbf{u}_h^\theta + \nabla p_h^\theta) \cdot \mathbf{w}(\mathbf{v}_h, q_h) dx \end{array} \right\}$$

Theorem

Bochev, Gunzburger, Shadid, CMAME 193, 2004

$$\sup_{\mathbf{v}_h, q_h \in V_h \times S_h} \frac{Q(\mathbf{u}_h, p_h; \mathbf{v}_h, q_h)}{\|\{\mathbf{v}_h, q_h\}\|_h} \geq \left(\frac{h^2}{4\Delta t C_I} + C_1(\theta, \Delta t, \tau) \right) \|\mathbf{u}_h\|_1 + C_2(\theta, \Delta t, \tau) \|\nabla p_h\|_0$$

$$C_2(\theta, \Delta t, \tau) = \frac{1}{2} \left\{ \begin{array}{ll} \tau(\theta - \tau\Delta t^{-1}) & \text{SGLS} \\ \tau(\theta - \tau\Delta t^{-1}/2) & \text{GLS} \\ \tau(\theta(1 - \gamma^{-1}) - \tau\Delta t^{-1}/2) & \text{RGLS} \end{array} \right\} \longrightarrow h^2 \leq C(\theta) \frac{\Delta t}{\delta}$$

- Appears in context of other stabilized methods (Codina, CMAME 182, 2000)
- *Sufficient* but not *necessary* stability condition
- Does not reveal the *mechanism* that may *corrupt* the pressure



Algebraic analysis

Linear algebra is messy, we restrict attention to

- Pressure-Poisson stabilization
- Uniform definition of the stabilization parameter: $\tau = \delta h^2$
- Implicit Euler time stepping: $\theta = 0$

Fully discrete equations

$$\left\{ \begin{array}{l} (\mathbf{u}_h^{k+1}, \mathbf{v}_h) \\ -\tau \sum_K \int_K \mathbf{u}_h^{k+1} \cdot \nabla q_h dx \end{array} \right\} + \Delta t \left\{ \begin{array}{l} a(\mathbf{u}_h^{k+1}, \mathbf{v}_h) - b(p_h^{k+1}, \mathbf{v}_h) - b(q_h, \mathbf{u}_h^{k+1}) \\ -\tau \sum_K \int_K (-\Delta \mathbf{u}_h^{k+1} + \nabla p_h^{k+1} - \mathbf{f}^{k+1}) \cdot \nabla q_h dx \end{array} \right\} = (\mathbf{f}_h^{k+1}, \mathbf{v}_h)$$

Algebraic system

$$\begin{pmatrix} M + \Delta t A \\ \tau B - \Delta t B - \tau \Delta t S \end{pmatrix} \begin{pmatrix} \mathbf{u}^{k+1} \\ p^{k+1} \end{pmatrix} = \begin{pmatrix} M & 0 \\ \tau B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u}^k \\ p^k \end{pmatrix} + \Delta t \begin{pmatrix} F^{k+1} \\ \tau G^{k+1} \end{pmatrix}$$

Solution

After tedious manipulations

$$\mathbf{u}^{k+1} = (M + \Delta t A)^{-1} \left[\begin{aligned} & \left(M - B^T (\tau K + \hat{G} B^T)^{-1} (\hat{G} M + \tau B) \right) \mathbf{u}^k + \\ & \Delta t \left(F^{k+1} - B^T (\tau K + \hat{G} B^T)^{-1} (\hat{G} F^{k+1} + \tau G^{k+1}) \right) \end{aligned} \right]$$

$$p^{k+1} = \frac{1}{\Delta t} (\tau K + \hat{G} B^T)^{-1} \left[(\hat{G} M + \tau B) \mathbf{u}^k + \Delta t \hat{G} F^{k+1} + \tau \Delta t G^{k+1} \right]$$

$$\hat{G} = [(\Delta t - \tau) B + \tau \Delta t S] (M + \Delta t A)^{-1}$$

Check: $\tau \rightarrow 0$ limit is as expected (Unstabilized Mixed Method)

$$\mathbf{u}^{k+1} = \left(I - M^{-1} B^T (B M^{-1} B^T)^{-1} \right) \mathbf{u}^k + O(\Delta t)$$

$$p^{k+1} = \frac{1}{\Delta t} (B M^{-1} B^T)^{-1} B \mathbf{u}^k + O(1)$$

Anatomy of the pressure-Poisson matrix

Velocity equation

$(M + \Delta t A) \rightarrow$ Cannot cause any trouble

Pressure equation

$$\begin{aligned} \tau K + \hat{G}B^T &= \Delta t B(M + \Delta t A)^{-1} B^T && \rightarrow \text{From Galerkin mixed form} \\ &+ \tau K && \rightarrow \text{Pressure-Poisson stabilization term} \\ &- \tau B(M + \Delta t A)^{-1} B^T && \rightarrow \text{Consistency term } (\dot{\mathbf{u}}, \nabla q) \\ &+ \tau \Delta t S(M + \Delta t A)^{-1} B^T && \rightarrow \text{Consistency term } (-\Delta \mathbf{u}, \nabla q) \end{aligned}$$

Confirms earlier analysis (sufficient stability condition)

$$\tau K + \hat{G}B^T = \underbrace{(\Delta t - \tau)}_{\text{unstable}} \underbrace{B(M + \Delta t A)^{-1} B^T}_{\text{stable}} + \tau K + O(\tau \Delta t)$$

$\Delta t - \tau > 0 \rightarrow$ Sufficient stability condition $\rightarrow h^2 \leq \frac{\Delta t}{\delta}$

The $\Delta t \rightarrow 0$ limit for fixed h

Theorem

$$\mathbf{u}^{k+1} = \mathbf{u}^k + O(\Delta t)$$

$$p^{k+1} = (K - BM^{-1}B^T)^{-1} \left[\frac{1}{\tau} B\mathbf{u}^k + (S + BM^{-1}A)\mathbf{u}^k - BM^{-1}F^{k+1} + G^{k+1} \right] + O(\Delta t)$$

Corollary

- Velocity *unaffected* at the small time step limit
- Pressure *can be corrupted* in two possible ways

$$p^{k+1} \approx (K - BM^{-1}B^T)^{-1} \left[\frac{1}{\tau} B\mathbf{u}^k \right] + O(\Delta t)$$

stable - **unstable**

Makes stability *unpredictable*

$B\mathbf{u}^k \neq 0$

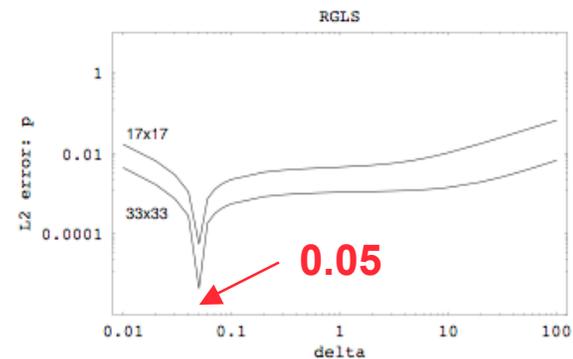
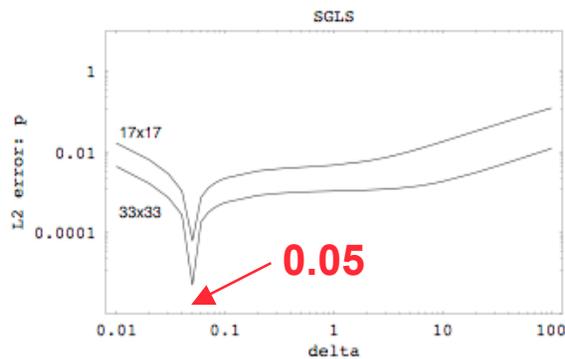
Makes pressure *dependent* on δ !



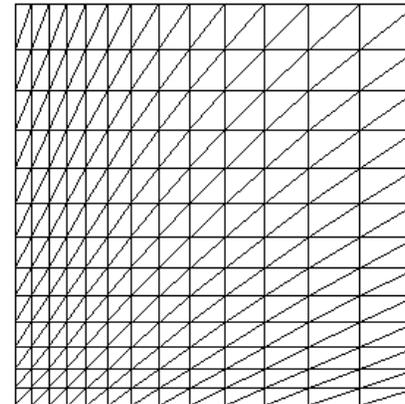
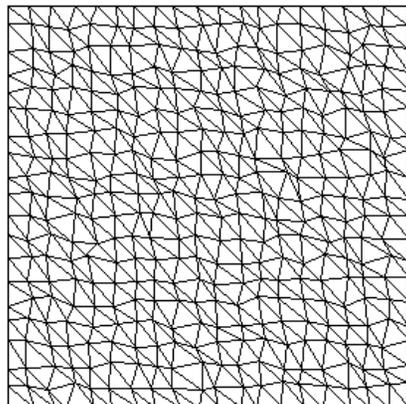
Numerical studies

SGLS/RGLS compared with Taylor-Hood

– For stationary equations both stable for any $\delta > 0$ (SGLS: *Bochev, Gunzburger, SINUM 2004*)



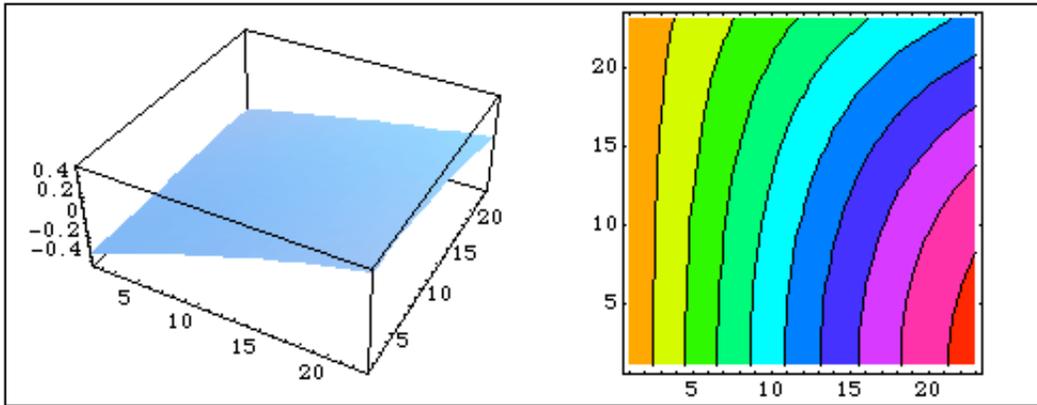
- Several values of δ , including an optimal one (*Barth, Bochev, Gunzburger, Shadid SISC 2003*)
- P2-P2 and P3-P3 elements on uniform and non-uniform grids





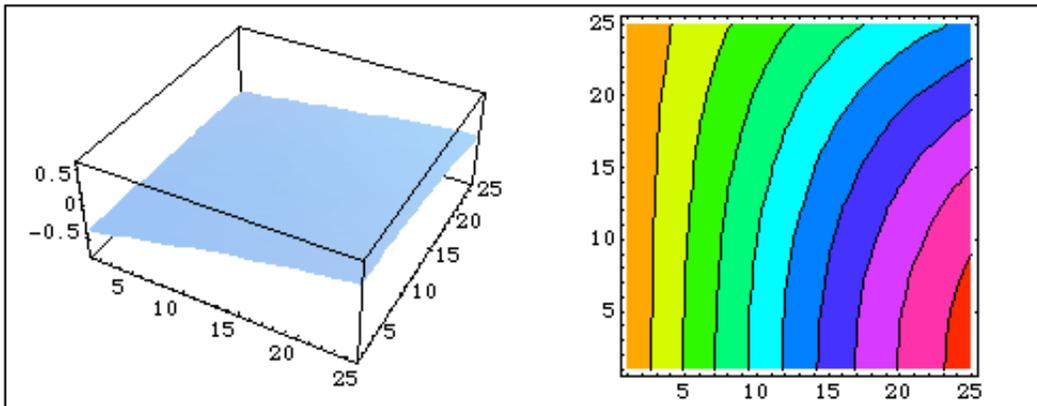
Taylor-Hood

20x20



Taylor-Hood dt=0.0000001

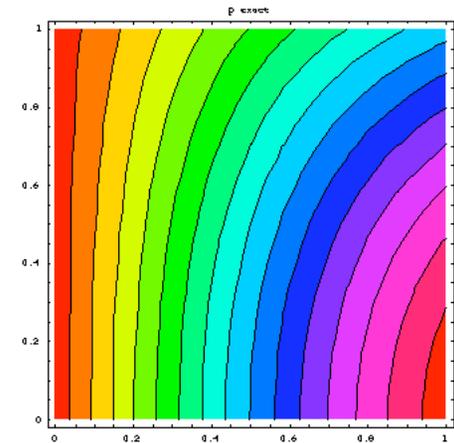
23x23 Random



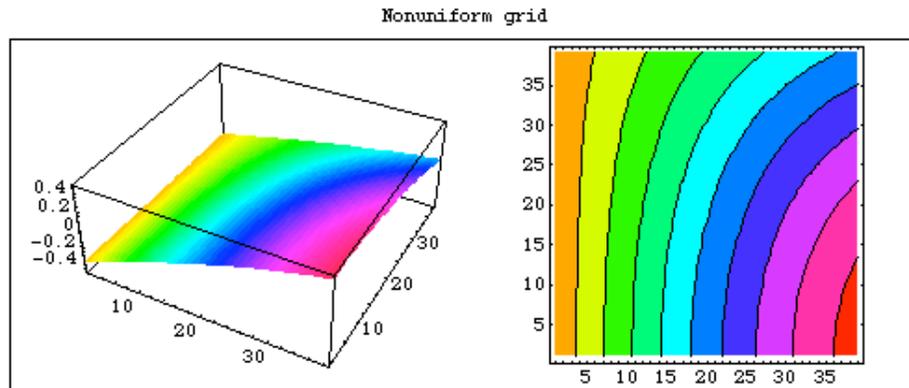
Taylor-Hood dt=0.0000001

Steady-state solution

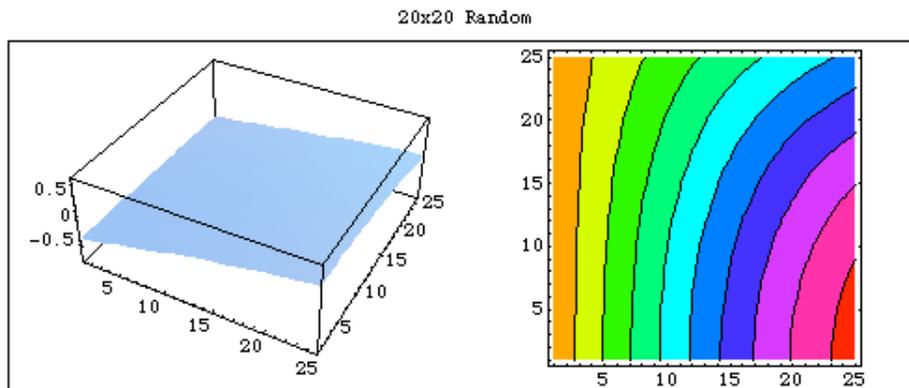
Elements	968
Unknowns	4226
Δt	10^{-7}
time steps	10^3



P2-P2 SGLS with optimal δ



Stabilized Galerkin



SGLS delta=0.05 dt=0.0000001

Uniform mesh

Elements P2-P2	722
Unknowns	4258
Δt	10^{-7}
time steps	10^{+3}
δ	0.05

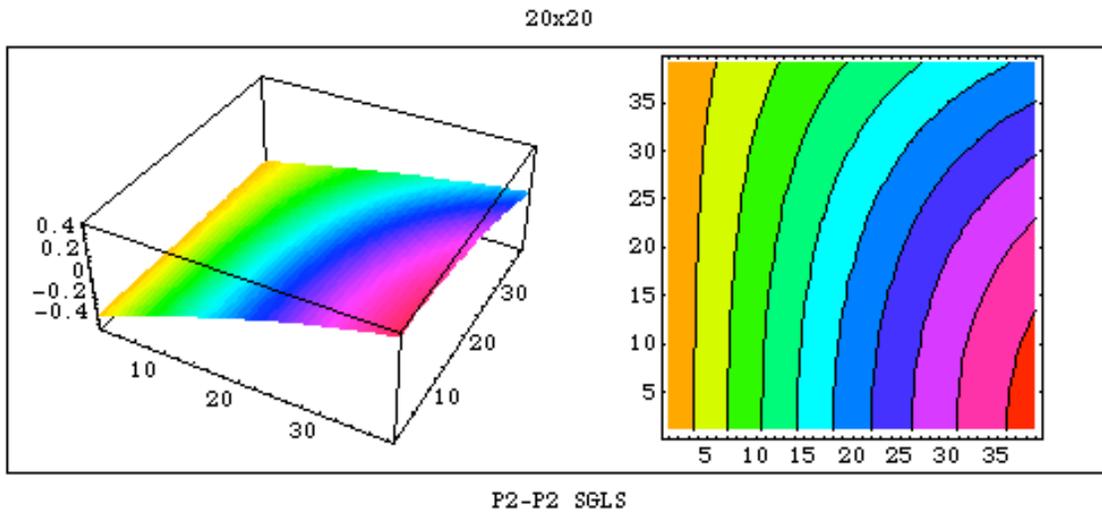
Random mesh

Elements P2-P2	722
Unknowns	4258
Δt	10^{-7}
time steps	10^{+3}
δ	0.05

- **Pressure exhibits spurious transient, recovers in 30-40 steps**
- **Velocity approximation not affected at all**



P2-P2 SGLS with $\delta < \delta_{opt}$



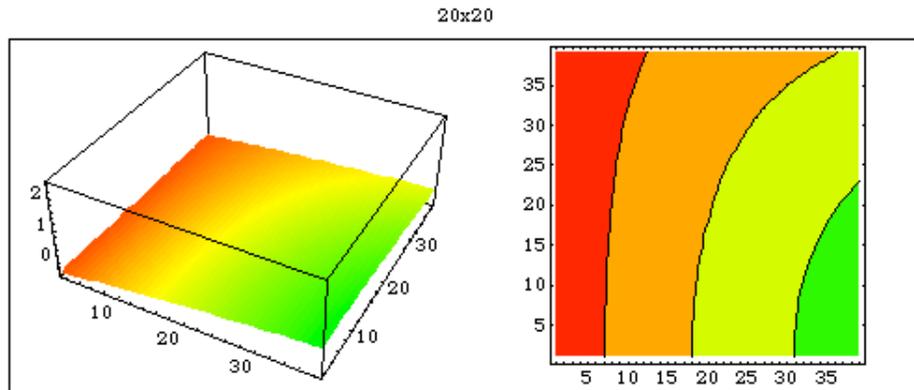
Uniform mesh

Elements	722
Unknowns	4258
Δt	10^{-7}
time steps	10^{+3}
δ	0.005

- Reducing δ takes the method back to mixed Galerkin formulation
- Pressure starts exhibiting node-to-node oscillations
- **Spurious transient is virtually eliminated**

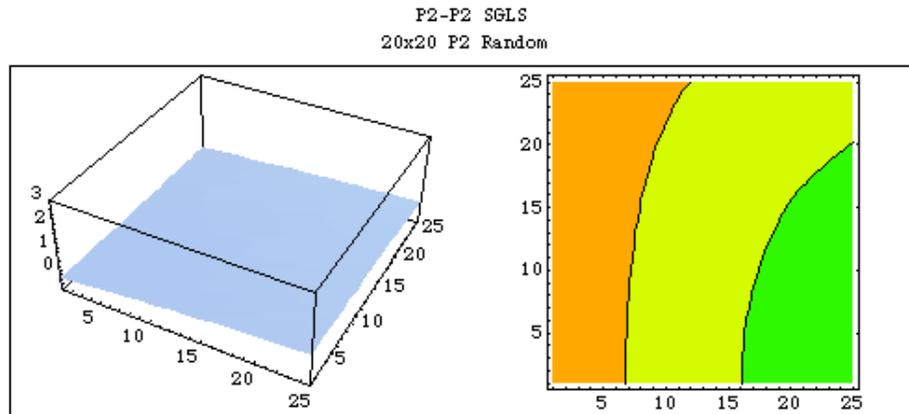


P2-P2 SGLS with $\delta > \delta_{opt}$



Uniform mesh

Elements P2-P2	722
Unknowns	4258
Δt	10^{-7}
time steps	10^{+3}
δ	5



Random mesh

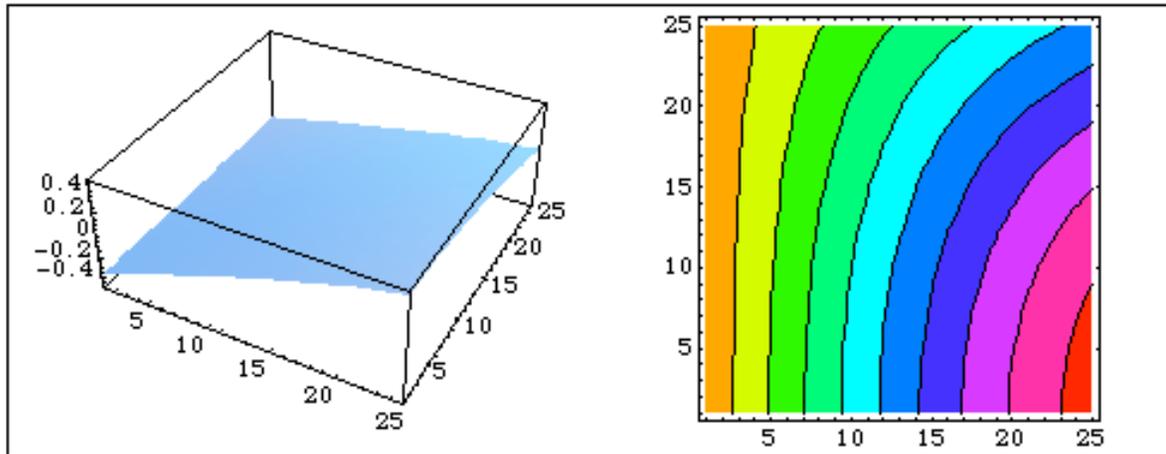
Elements P2-P2	722
Unknowns	4258
Δt	10^{-7}
time steps	10^{+3}
δ	5

- Pressure spurious transient takes longer to recover
- Velocity approximation does not seem affected



Is P3-P3 better?

14x14 random

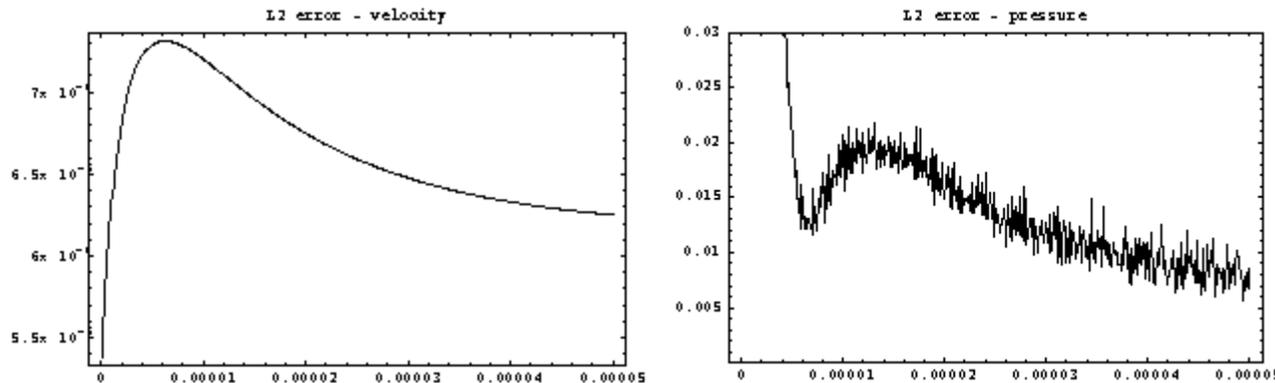


Random mesh

Elements **P3-P3** 338
Unknowns 4487
 Δt 10^{-7}
time steps 10^3
 δ **0.05**

P3 SGLS dt=0.0000001, nt=500

SGLS

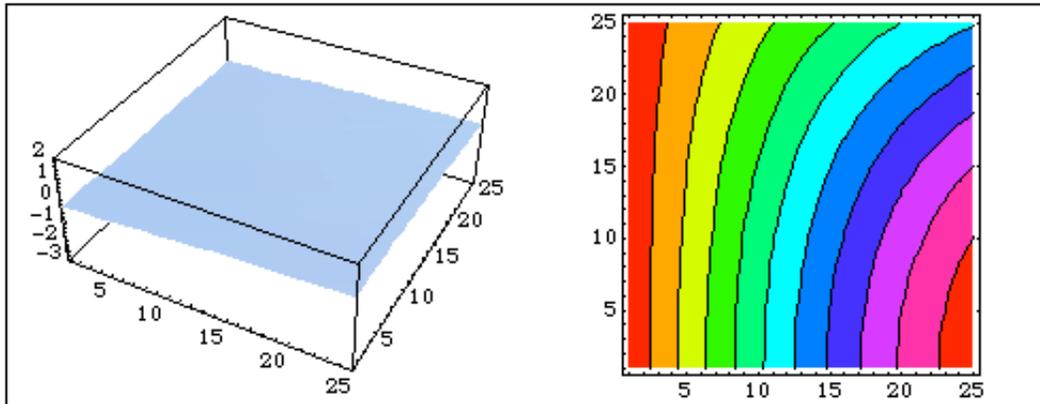


– High-frequency noise, induced by grid topology, persists!



P3-P3 SGLS with $\delta > \delta_{opt}$

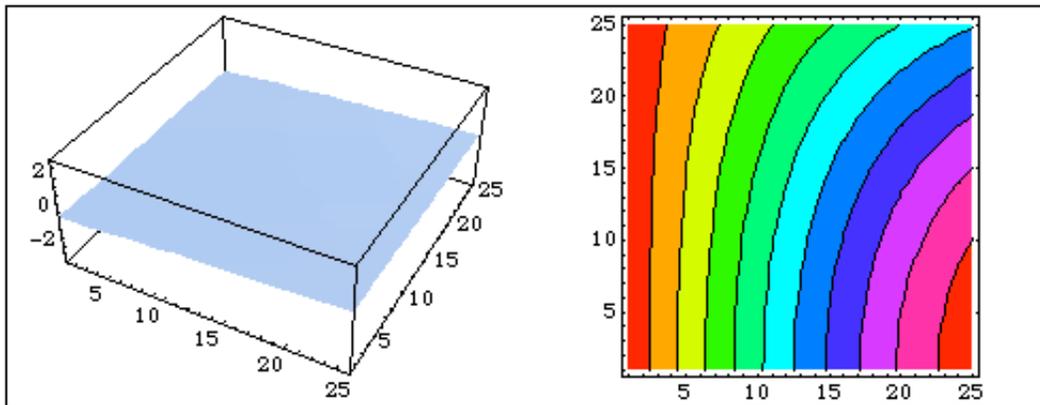
14x14 P3 Non-uniform



Non-uniform mesh

Elements P3-P3	338
Unknowns	4487
Δt	10^{-7}
time steps	10^{+3}
δ	5

14x14 P3 Random



Random mesh

Elements P3-P3	338
Unknowns	4487
Δt	10^{-7}
time steps	10^{+3}
δ	5

SGLS delta=5 dt=0.0000001, nt=1000

- Spurious transient persists - pressure does not appear to recover
- For random mesh errors begin to grow, including in *velocity*!



Conclusions

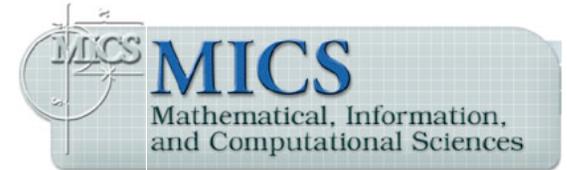
- Small time steps are a *challenge* for spatially stabilized formulations
- Computations *sensitive* to
 - Grid topology
 - Stabilization parameter
- Range of τ may have to be additionally *restricted*

A possible explanation:

Separated discretization applies multiscale effects to spatial discretization only, *time scales* not treated *consistently* with *spatial scales*

Possible remedies

- Time-space formulations (how to justify for Stokes where we deal with a purely spatial constraint?)
- Non-residual stabilization



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Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

