MICS
Mathematical, Information, and Computational Sciences

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

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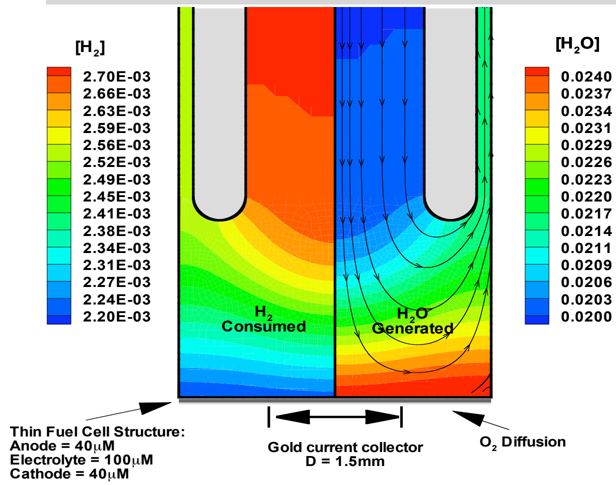
Problems with multiple time scales at Sandia: MP Salsa, CHARON

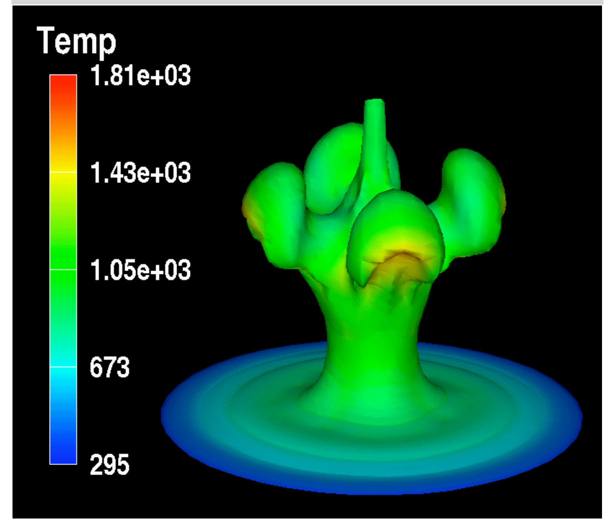
Applications:

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

Simulation of Experimental Solid Oxide Fuel Cell

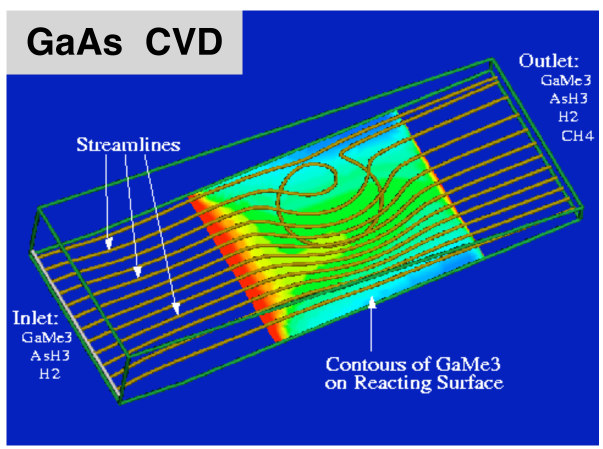


Turbulent Combustion Simulation Of Methanol Pool Fire

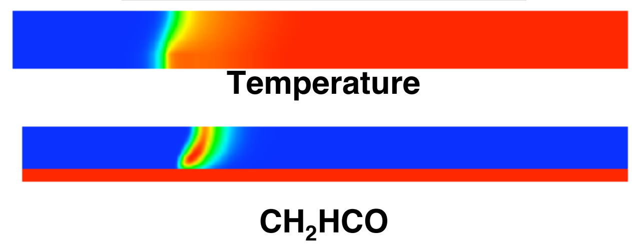


Processes

- ➢ Chemical kinetics
- ➢ Momentum diffusion
- ➢ Heat conduction
- ➢ Convection



Ethane Catalysis



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Model equations and their discretization

PDE Model

$$\begin{Bmatrix} \rho\dot{\mathbf{u}} - \nabla\cdot\mathbf{T} + \rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \rho\mathbf{g} \\ \nabla\cdot(\rho\mathbf{u}) = 0 \end{Bmatrix} + \begin{Bmatrix} \text{species fraction} \\ \text{thermal energy} \end{Bmatrix}$$

Discrete equations

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

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

- *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

Hughes, Hulbert, Franca, Shakib, Jansen, Collis, Tezdyar, 1986 -

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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!

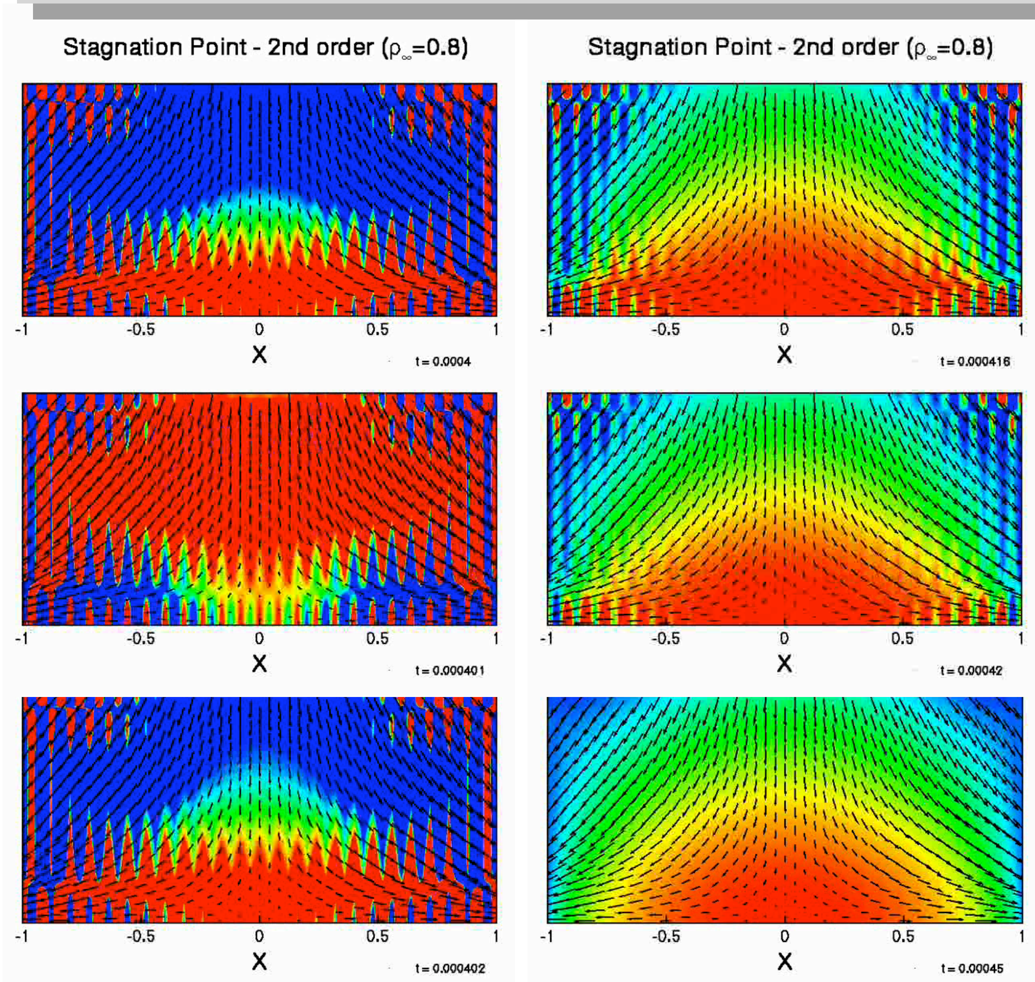
Time integration issues

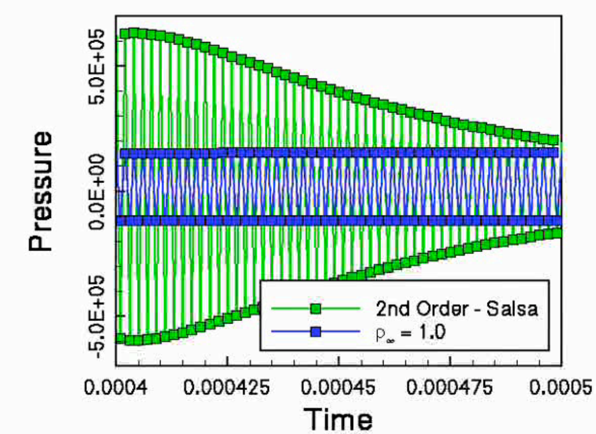
- Application of *operator-split* methods accompanied by *instabilities* due to the complex multiphysics (*Shadid, Ropp, Ober, JCP 2004*)
- *Fully implicit* solvers and *physics based* preconditioners preferred for *stability* and stiff diffusion terms
- Resolving non-equilibrium chemical reaction requires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

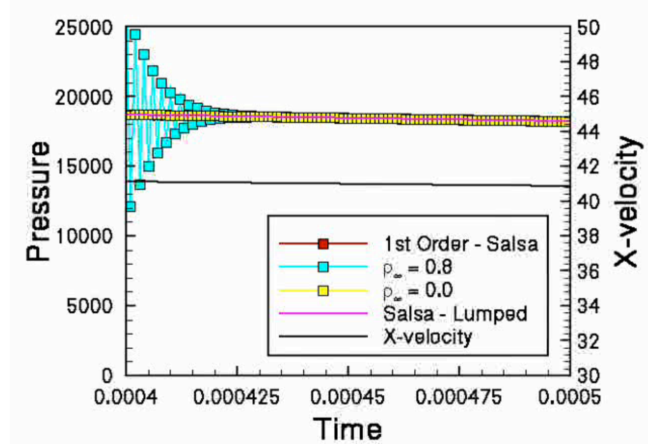
C. Ober, J. Shadid, unpublished

Pressure instabilities: MP Salsa

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



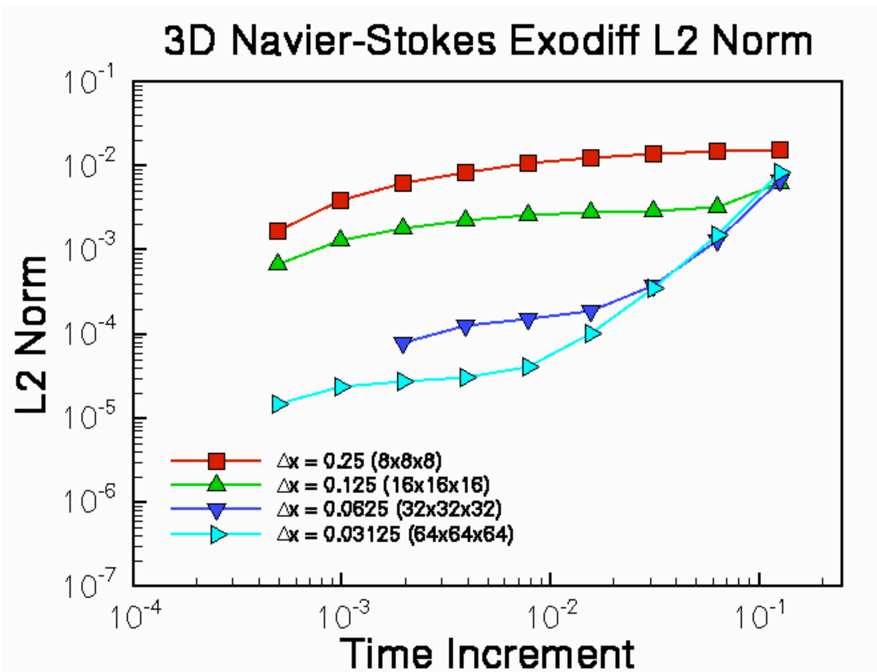




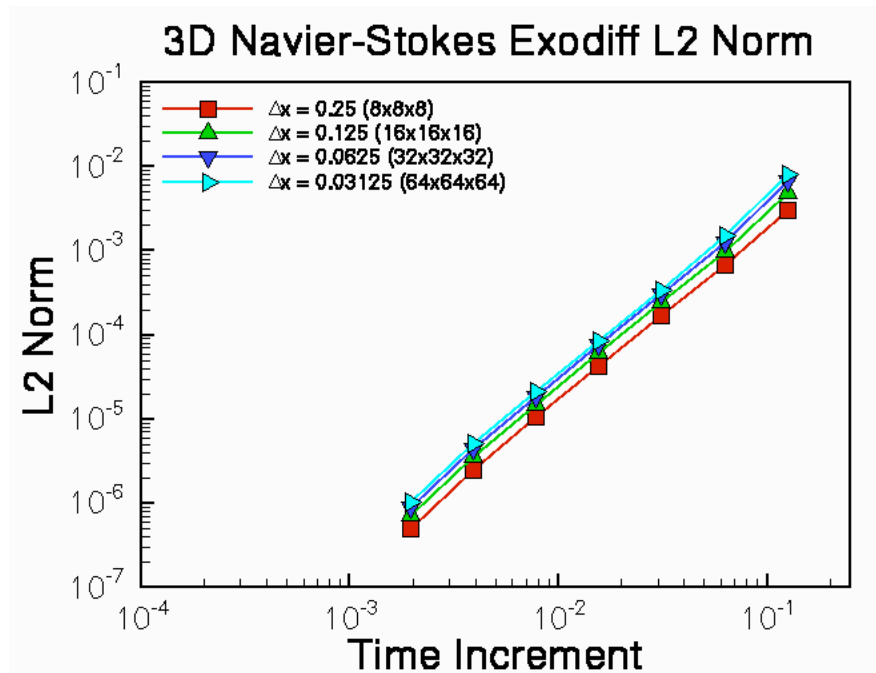
Convergence stagnation

Analytic 3D Navier-Stokes Solution

Δt included in τ



Δt removed from τ



Modification of τ helped to offset stagnation.

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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:

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

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

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

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

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

Theorem

Bochev, Gunzburger, Shadid, CMAME 193, 2004

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

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

– 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

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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

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

Algebraic system

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

Solution

After tedious manipulations

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

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

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

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

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

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

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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)

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

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

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

Theorem

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

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

Corollary

– Velocity *unaffected* at the small time step limit

– Pressure *can be corrupted* in two possible ways

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

stable - unstable

Makes stability *unpredictable*

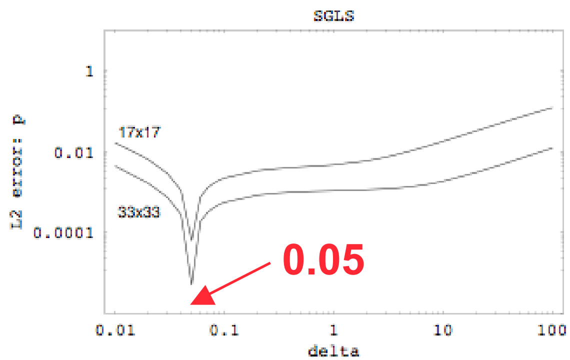
$B\mathbf{u}^k \neq 0$

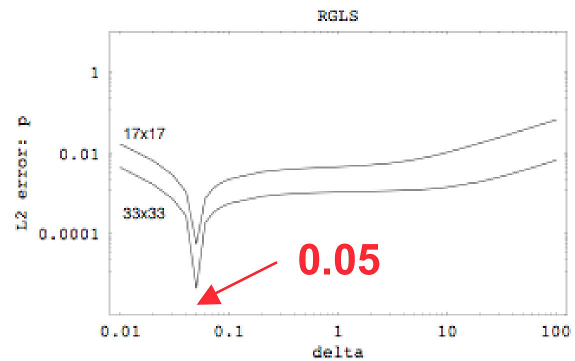
Makes pressure *dependent* on δ!

Numerical studies

SGLS/RGLS compared with Taylor-Hood

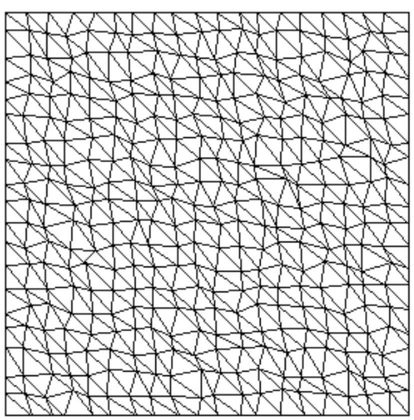
– For stationary equations both stable for any $\delta>0$ (SGLS: *Bochev, Gunzburger, SINUM 2004*)

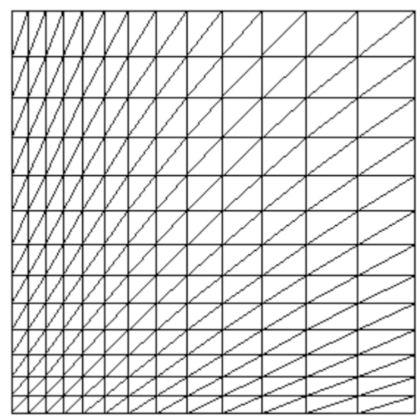




– Several values of δ, including an optimal one (*Barth, Bochev, Gunzburger,Shadid SISC 2003)*

– P2-P2 and P3-P3 elements on uniform and non-uniform grids





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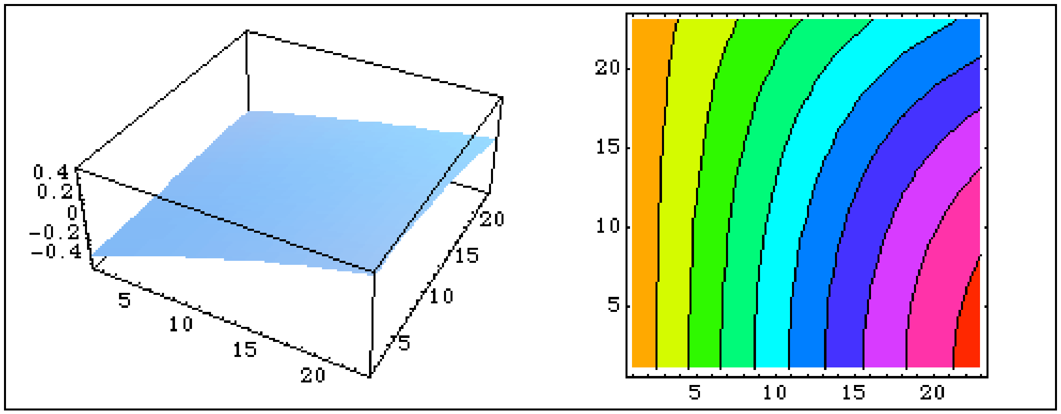
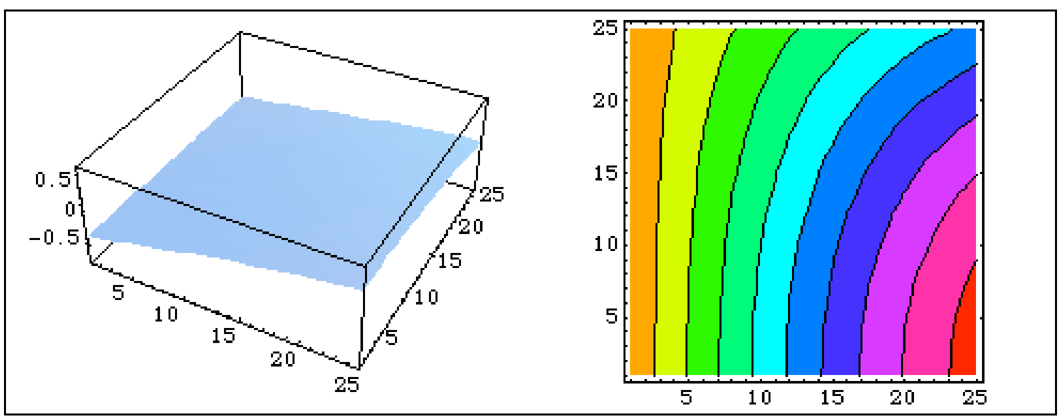
Taylor-Hood

20x20



Taylor-Hood dt=0.0000001

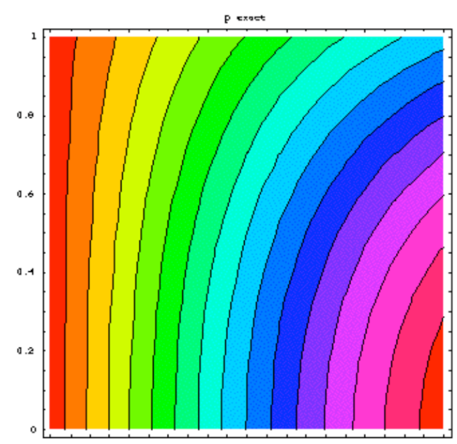
23x23 Random



Taylor-Hood dt=0.0000001

Steady-state solution

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



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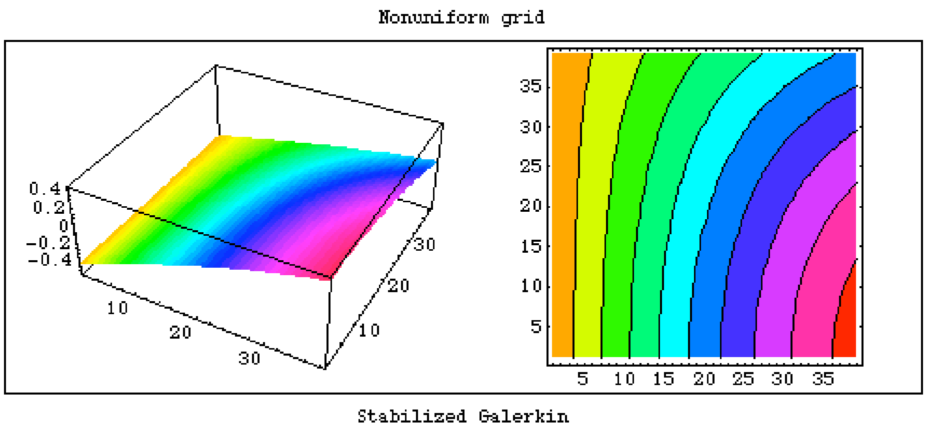
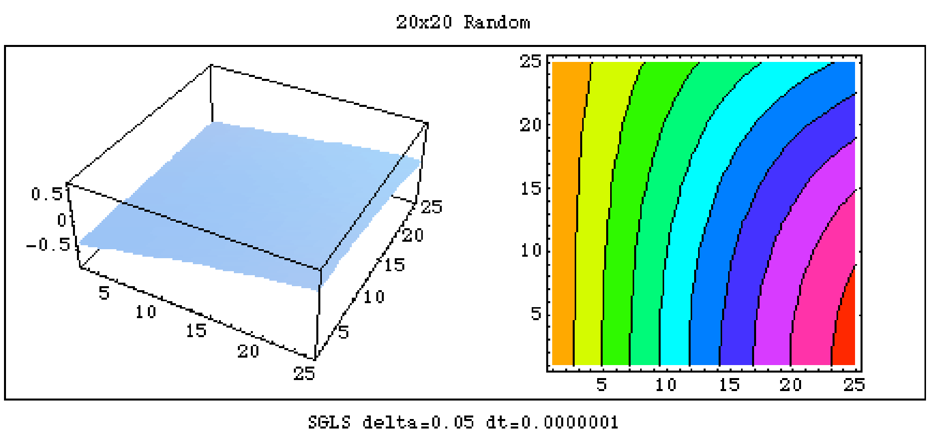
P2-P2 SGLS with optimal δ



Uniform mesh

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

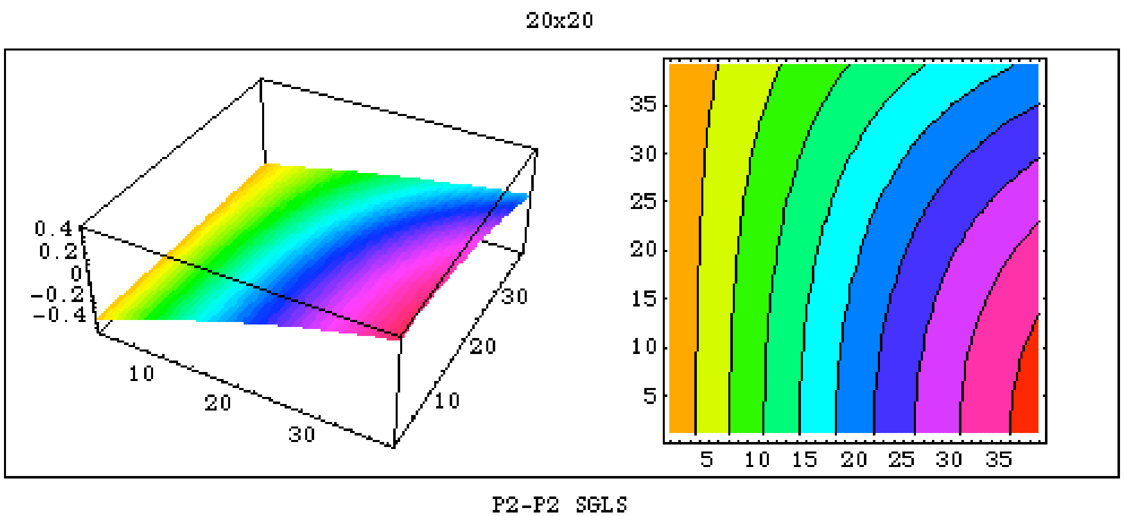


Random mesh

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**

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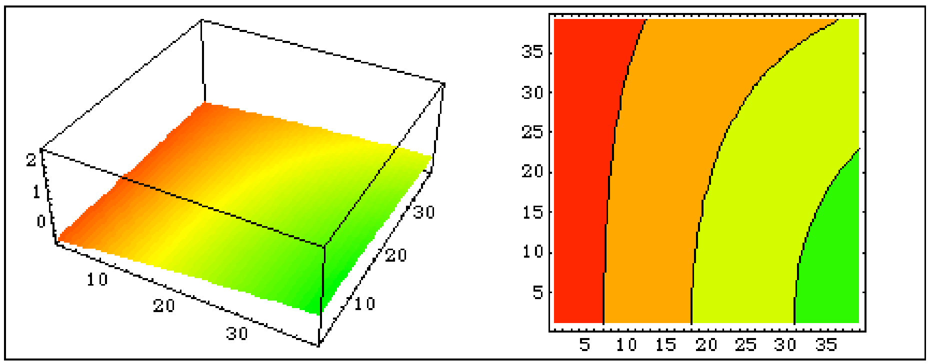
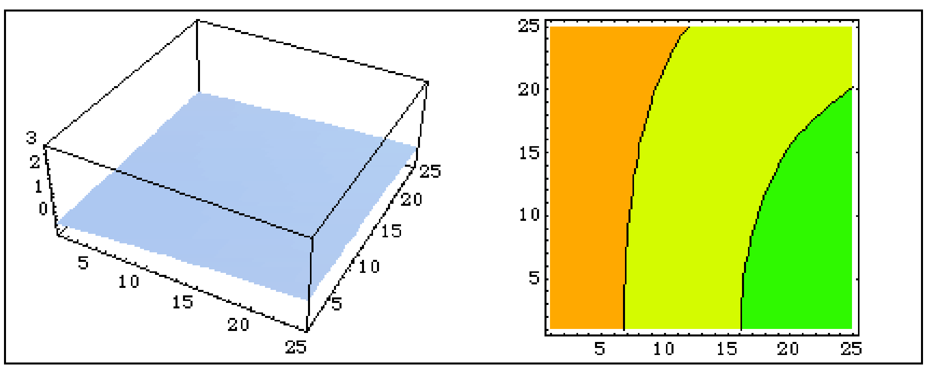
P2-P2 SGLS with $\delta > \delta_{opt}$

20x20



P2-P2 SGLS

20x20 P2 Random



SGLS delta=5 dt=0.0000001

Uniform mesh

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

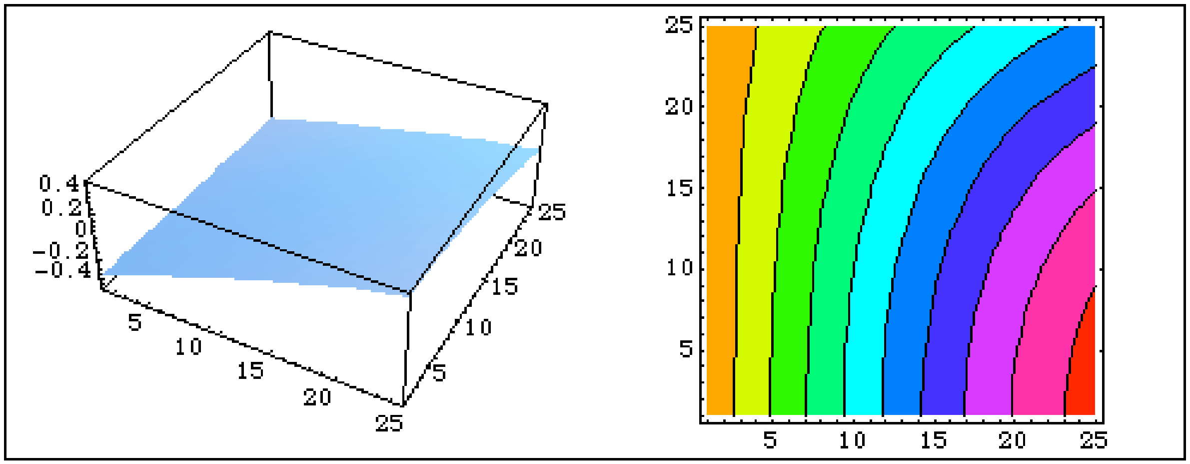
Random mesh

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

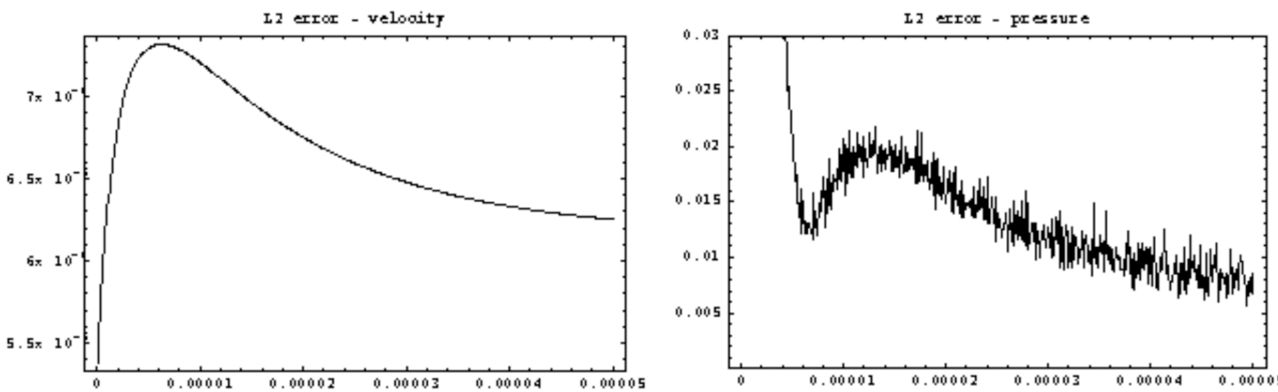
- **Pressure spurious transient takes longer to recover**
- **Velocity approximation does not seem affected**

Is P3-P3 better?

14x14 random



P3 SGLS dt=0.0000001, nt=500



Random mesh

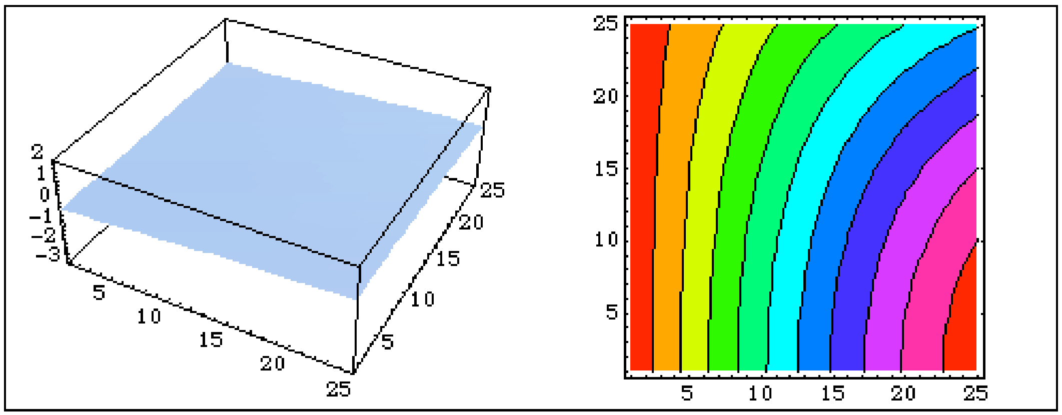
Elements **P3-P3**	338
Unknowns	4487
Δt	10^{-7}
time steps	10^{+3}
δ	**0.05**

SGLS

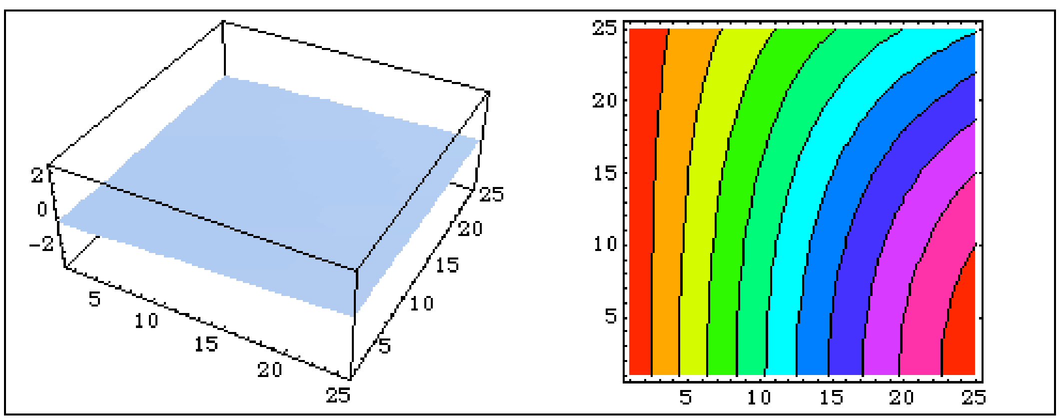
– **High-frequency noise, induced by grid topology, persists!**

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

14x14 P3 Non-uniform



14x14 P3 Random



SGLS delta=5 dt=0.0000001, nt=1000

Non-uniform mesh

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

Random mesh

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

- **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