Numerical Approximation of Complex Fluids

Noel Walkington

Department of Mathematical Sciences
Carnegie Mellon University
Pittsburgh, PA, USA

January 12, 2009

Fluid Mixtures

Momentum Equation: (weak form)

$$\int_\Omega (\rho\dot{v}, w) - (p, div(w)) + \mu(D(v), D(w)) + (T_e, \nabla w) = \int_\Omega \rho f.w$$

Elastic Energy and Stress: $\mathcal{W} = \mathcal{W}(\phi, \nabla\phi)$ and $T_e = \nabla\phi \otimes \dfrac{\partial \mathcal{W}}{\partial \nabla\phi}$

Transport of the Internal Variable: (with dissipation $\gamma \geq 0$)

$$\dot{\phi} \equiv \phi_t + v.\nabla\phi = -\gamma\frac{\delta\mathcal{W}}{\delta\phi} \equiv -\gamma\left(\frac{\partial\mathcal{W}}{\partial\phi} - div\left[\frac{\partial\mathcal{W}}{\partial\nabla\phi}\right]\right)$$

Energy Estimate:

$$\frac{d}{dt}\int_\Omega ((\rho/2)|v|^2 + \mathcal{W}) + \int_\Omega (\mu|D(v)|^2 + \gamma|\delta\mathcal{W}/\delta\phi|^2) = \int_\Omega \rho f.v$$

Energy Estimate & Galerkin Approximations

Reformulate the Elastic Stress: $div(T_e) = \dots$

$$\int_\Omega (\rho\dot{v}, w) - (p, div(w)) + \mu(D(v), D(w)) - (1/\gamma)(\dot{\phi}, \nabla\phi.w) = \int_\Omega \rho f.w$$

Transport Equation: (weak form)

$$\int_\Omega (1/\gamma)\dot{\phi}\psi + \frac{\partial\mathcal{W}}{\partial\phi}\psi + \left(\frac{\partial\mathcal{W}}{\partial\nabla\phi}\right).\nabla\psi = 0$$

Energy Estimate:

- Set $w = v$ in the momentum equation
- Set $\psi = \phi_t$ in the transport equation

$$\frac{d}{dt}\int_\Omega ((\rho/2)|v|^2 + \mathcal{W}) + \int_\Omega \left(\mu|D(v)|^2 + (1/\gamma)|\dot{\phi}|^2\right) = \int_\Omega \rho f.v$$

Evolution Equations

Abstract Equation: $u : [0, T] \to U$, satisfies $u(0) = u_0$

$$u_t + A(u) = F(u) \qquad \text{in } U'$$

Evolution Equations

Abstract Equation: $u : [0, T] \to U$, satisfies $u(0) = u_0$

$$u_t + A(u) = F(u) \qquad \text{in } U'$$

Abstract Weak Statement: $U \hookrightarrow H \hookrightarrow U'$

$$(u_t, v)_H + a(u, v) = \langle F(u), v\rangle \qquad v \in U$$

- U is a Banach Space, H is a Hilbert space, $U \hookrightarrow H$
- $a : U \times U \to \mathbb{R}$ is coercive, $a(u, u) \geq c_a\|u\|_U^p$
- $F : U \to U'$

Note: The operators may depend explicity upon time.

Evolution Equations

Abstract Equation: $u : [0, T] \to U$, satisfies $u(0) = u_0$

$$u_t + A(u) = F(u) \qquad \text{in } U'$$

Abstract Weak Statement: $U \hookrightarrow H \hookrightarrow U'$

$$(u_t, v)_H + a(u, v) = \langle F(u), v \rangle \qquad v \in U$$

Energy Estimate: Set $v = u$ and integrate in time

$$\frac{1}{2}\|u(t)\|_H^2 + \int_0^t c_a \|u\|_U^p \leq \frac{1}{2}\|u_0\|_H + \int_0^t \langle F(u), u \rangle.$$

Bounds: $u \in L^\infty[0, T; H] \cap L^p[0, T; U]$

Notation: $\|u\|_{L^p[0,T;U]} = \left(\int_0^T \|u(t)\|_U^p \, dt \right)^{1/p}$

Evolution Equations

Abstract Equation: $u : [0, T] \to U$, satisfies $u(0) = u_0$

$$u_t + A(u) = F(u) \qquad \text{in } U'$$

Abstract Weak Statement: $U \hookrightarrow H \hookrightarrow U'$

$$(u_t, v)_H + a(u, v) = \langle F(u), v\rangle \qquad v \in U$$

Energy Estimate: Set $v = u$ and integrate in time

$$\frac{1}{2}\|u(t)\|_H^2 + \int_0^t c_a \|u\|_U^p \le \frac{1}{2}\|u_0\|_H + \int_0^t \langle F(u), u\rangle.$$

Alternative Estimate: If $A = D\Phi$, set $v = u_t$

$$\int_0^t \|u_t\|_H^2 + \Phi(u(t)) \le \Phi(u_0) + \int_0^t (F(u), u_t)_H.$$

Bounds: $u_t \in L^2[0, T; H]$, $u \in L^\infty[0, T; U]$

Numerical Approximations

Discrete Spaces: Let $U_h \subset U$ be finite dimensional

Semi-Discrete Galerkin Approximation: $u_h : [0, T] \to U_h$

$$(u_{ht}, v_h)_H + a(u_h, v_h) = \langle F(u_h), v_h \rangle \qquad v_h \in U_h$$

This is a system of ordinary differential equations.

Numerical Approximations

Discrete Spaces: Let $U_h \subset U$ be finite dimensional

Semi-Discrete Galerkin Approximation: $u_h : [0, T] \to U_h$

$$(u_{ht}, v_h)_H + a(u_h, v_h) = \langle F(u_h), v_h \rangle \qquad v_h \in U_h$$

This is a system of ordinary differential equations.

Energy Estimate (Stability): Set $v_h = u_h$

$$\frac{1}{2}\|u_h(t)\|_H^2 + \int_0^t c_a \|u_h\|_U^p \leq \frac{1}{2}\|u_0\|_H + \int_0^t \langle F(u_h), u_h \rangle.$$

Alternatively: If $A = D\Phi$, set $v_h = u_{ht}$

$$\int_0^t \|u_h\|_H^2 + \Phi(u) \leq \Phi(u_0) + \int_0^t (F(u_h), u_{ht})_H.$$

Numerical Approximations

Discrete Spaces: Let $U_h \subset U$ be finite dimensional

Semi-Discrete Galerkin Approximation: $u_h : [0, T] \to U_h$

$$(u_{ht}, v_h)_H + a(u_h, v_h) = \langle F(u_h), v_h \rangle \qquad v_h \in U_h$$

This is a system of ordinary differential equations.

Question: What is a "good" time stepping scheme?

Numerical Approximations

Discrete Spaces: Let $U_h \subset U$ be finite dimensional

Semi-Discrete Galerkin Approximation: $u_h : [0, T] \to U_h$

$$(u_{ht}, v_h)_H + a(u_h, v_h) = \langle F(u_h), v_h \rangle \qquad v_h \in U_h$$

This is a system of ordinary differential equations.

Question: What is a "good" time stepping scheme?

Rule of Thumb

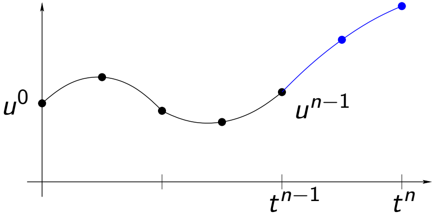
- If stability follows upon setting $v = u$ then use DG

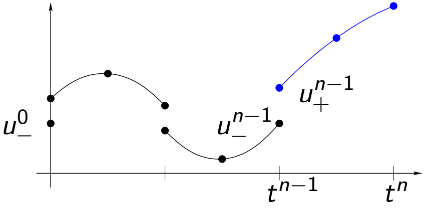
  Lowest order DG scheme is implicit Euler
- If stability follows upon setting $v = u_t$ then use CG

  Lowest order CG scheme is the trapezoid rule

Time Stepping Schemes

Time Partition: $0 = t^0 < t^1 < \ldots < t^N = T$



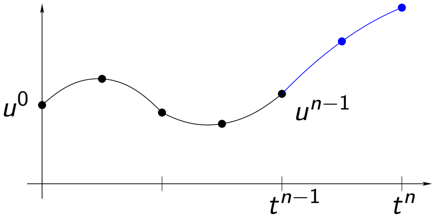


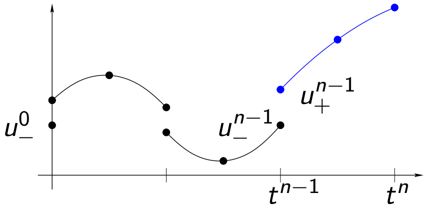
CG Time Stepping Scheme

DG Time Stepping Scheme

Time Stepping Schemes

Time Partition: $0 = t^0 < t^1 < \ldots < t^N = T$





CG Time Stepping Scheme   DG Time Stepping Scheme

CG Scheme: $u_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$ satisfies $u_h(t_+^{n-1}) = u_h(t_-^{n-1})$ and

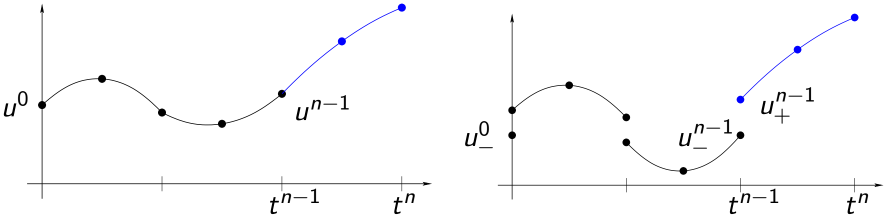
$$\int_{t^{n-1}}^{t^n} \Big((u_{ht}, v_h)_H + a(u_h, v_h) \Big) = \int_{t^{n-1}}^{t^n} \langle F(u_h), v_h \rangle$$

for all $v_h \in \mathcal{P}_{\ell-1}[t^{n-1}, t^n; U_h]$

Stability: Set $v_h = u_{ht} \in \mathcal{P}_{\ell-1}[t^{n-1}, t^n; U_h] \ldots$

Time Stepping Schemes

Time Partition: $0 = t^0 < t^1 < \ldots < t^N = T$



CG Time Stepping Scheme DG Time Stepping Scheme

DG Scheme: $u_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$

$$\int_{t^{n-1}}^{t^n} \Big((u_{ht}, v_h)_H + a(u_h, v_h) \Big) + ([u^{n-1}], v_+^{n-1})_H = \int_{t^{n-1}}^{t^n} \langle F(u_h), v_h \rangle$$

for all $v_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$

Notation: Jump term $[u^m] = u_+^m - u_-^m$

DG Time Stepping Scheme

DG Scheme: $u_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$

$$\int_{t^{n-1}}^{t^n} \Big((u_{ht}, v_h)_H + a(u_h, v_h) \Big) + ([u^{n-1}], v_+^{n-1})_H = \int_{t^{n-1}}^{t^n} \langle F(u_h), v_h \rangle$$

for all $v_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$

Energy Estimate (Stability): Set $v_h = u_h$

$$\frac{1}{2}\|u_-^n\|_H^2 + \frac{1}{2}\sum_{m=0}^{n-1} \|[u^m]\|_H^2 + \int_0^{t^n} c_a \|u_h\|_U^p \leq \frac{1}{2}\|u_-^0\|_H^2 + \int_0^{t^n} \langle F(u_h), u_h \rangle$$

Note: For $\ell > 1$ bounds in $L^\infty[0, T; H]$ are not automatic.

$$\max_{1 \leq n \leq N} \|u_-^n\|_H \leq C(u_-^0, F).$$

DG Time Stepping Scheme

DG Scheme: $u_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$

$$\int_{t^{n-1}}^{t^n} \Big((u_{ht}, v_h)_H + a(u_h, v_h) \Big) + ([u^{n-1}], v_+^{n-1})_H = \int_{t^{n-1}}^{t^n} \langle F(u_h), v_h \rangle$$

for all $v_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$

Energy Estimate (Stability): Set $v_h = u_h$

$$\frac{1}{2}\|u_-^n\|_H^2 + \frac{1}{2}\sum_{m=0}^{n-1} \|[u^m]\|_H^2 + \int_0^{t^n} c_a \|u_h\|_U^p \le \frac{1}{2}\|u_-^0\|_H^2 + \int_0^{t^n} \langle F(u_h), u_h \rangle$$

Convergence:

- Lax Equivalence Theorem: A (linear) numerical scheme converges if and only if it is stable and consistent.
- For nonlinear problems compactness is required to guarantee convergence of the nonlinear terms!

Compactness of Solutions

Theorem: (Lions-Aubin) *Let B_0, B and B_1 be Banach spaces satisfying $B_0 \hookrightarrow\!\!\!\!\rightarrow B \hookrightarrow B_1$ where the first inclusion is compact. If $0 < T < \infty$, $1 \leq p, q < \infty$, and*

$$W = W(0,T) = \{u \in L^p[0,T;B_0] \mid u_t \in L^q[0,T;B_1]\},$$

then the inclusion $W \hookrightarrow\!\!\!\!\rightarrow L^p[0,T;B]$ is compact.

Compactness of Solutions

Theorem: (Lions-Aubin) *Let B_0, B and B_1 be Banach spaces satisfying $B_0 \hookrightarrow\!\!\!\rightarrow B \hookrightarrow B_1$ where the first inclusion is compact. If $0 < T < \infty$, $1 \le p, q < \infty$, and*

$$W = W(0,T) = \{u \in L^p[0,T;B_0] \mid u_t \in L^q[0,T;B_1]\},$$

then the inclusion $W \hookrightarrow\!\!\!\rightarrow L^p[0,T;B]$ is compact.

Typical Application: Set $U \hookrightarrow H \hookrightarrow U'$

- For parabolic problems $U \hookrightarrow\!\!\!\rightarrow H$ is typically compact
- The energy estimate bounds u in $L^p[0,T;U]$
- To estimate the time derivative, write

$$\int_0^T (u_t, v) = \int_0^T \langle F(u), v\rangle - a(u,v)$$

Bounds on u and growth conditions on $F(.)$ and $a(.,.)$ are used to bound u_t in $L^q[0,T;U']$

Compactness of Solutions

Theorem: (Lions-Aubin) *Let B_0, B and B_1 be Banach spaces satisfying $B_0 \hookrightarrow\!\!\!\!\rightarrow B \hookrightarrow B_1$ where the first inclusion is compact. If $0 < T < \infty$, $1 \leq p, q < \infty$, and*

$$W = W(0, T) = \{u \in L^p[0, T; B_0] \mid u_t \in L^q[0, T; B_1]\},$$

then the inclusion $W \hookrightarrow\!\!\!\!\rightarrow L^p[0, T; B]$ is compact.

Problem: DG solutions are discontinuous so $u_{ht} \notin L^q[0, T, B_1]$

Compactness of Discrete Solutions

Theorem: (njw) *Let H be a Hilbert space, U a Banach space and $U \hookrightarrow\!\!\!\rightarrow H \hookrightarrow U'$ be dense compact embeddings. Fix $\ell \geq 0$ to be an integer, and $1 \leq p, q < \infty$. Let $h > 0$ be a (mesh) parameter and for each h let $\{t_h^i\}_{i=0}^{N_h}$ be a uniform partition of $[0, T]$ and $U_h \subset U$ be a subspace. Assume that*

1. *For each $h > 0$, $u_h|_{(t_h^{n-1}, t_h^n)} \in \mathcal{P}_\ell[t_h^{n-1}, t_h^n; U_h]$ and*

$$\int_{t_h^{n-1}}^{t_h^n} (u_{ht}, v_h)_H + ([u^{n-1}], v_+^{n-1})_H = \int_{t_h^{n-1}}^{t_h^n} \langle F_h, v_h \rangle,$$

   for each $v_h \in \mathcal{P}_\ell[t^{n-1}, t^n; U_h]$.

2. *$\{u_h\}_{h>0} \subset L^p[0, T; U]$ is bounded.*
3. *$\{F_h\}_{h>0} \subset L^q[0, T; U_h']$ is bounded.*

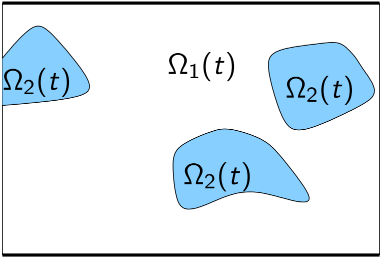
Compactness of Discrete Solutions

Theorem: (njw) *Let H be a Hilbert space, U a Banach space and $U \hookrightarrow\!\!\!\rightarrow H \hookrightarrow U'$ be dense compact embeddings. Fix $\ell \geq 0$ to be an integer, and $1 \leq p, q < \infty$. Let $h > 0$ be a (mesh) parameter and for each h let $\{t_h^i\}_{i=0}^{N_h}$ be a uniform partition of $[0, T]$ and $U_h \subset U$ be a subspace. Assume that ...*

Then,

1. *If $p > 1$ then $\{u_h\}_{h>0} \subset L^r[0, T; H]$ is compact for $1 \leq r < 2p$.*
2. *If $1 \leq 1/p + 1/q < 2$ and $\sum_{n=1}^{N_h} \|[u^n]\|_H^2$ is bounded independently of h then $\{u_h\}_{h>0} \subset L^r[0, T; H]$ is compact for $1 \leq r < 2/(1/p + 1/q - 1)$.*

Mixtures of Immiscible Fluids



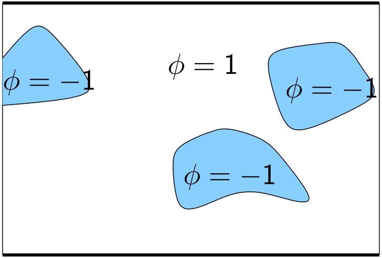
Weak Statement of the NS Equations and Interface Condition

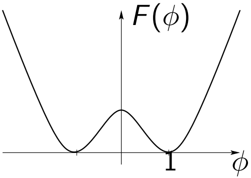
$$\int_\Omega \Big\{ (v_t + (v.\nabla)v, w) - (p, div(w)) \quad + \quad \nu(D(v), D(w)) \Big\}$$

$$+ \quad \int_{S(t)} \gamma H n.w = \int_\Omega f.w$$

Incompressibility Condition: $\int_\Omega div(v) q = 0$

Phase Field Approximations





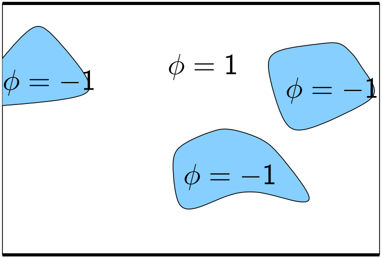
Phase Field Approximation: $S(t) = \{x \in \Omega \mid \phi(x) = 0\}$

Formal Asymptotics: Let $F(\phi) = (1/2)(\phi^2 - 1)^2$ then

$$\int_\Omega (1/\epsilon)(\epsilon\Delta\phi - (1/\epsilon)F'(\phi))\,\psi \simeq 2\int_{S(t)} \psi$$

$$\int_\Omega (\epsilon\Delta\phi - (1/\epsilon)F'(\phi))\nabla\phi.w \simeq (4/3)\int_{S(t)} Hn.w$$

Regularized Equations

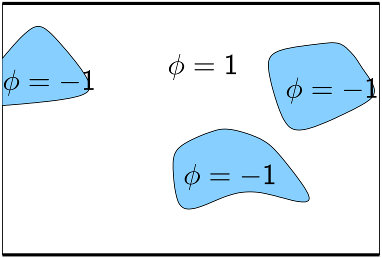


Momentum Equation

$$\int_\Omega \Big\{ (v_t + (v.\nabla)v, w) - (p, div(w)) + \nu(D(v), D(w)) + \gamma\left(\epsilon\Delta\phi - (1/\epsilon)F'(\phi), \nabla\phi.w\right)\Big\} = \int_\Omega f.w.$$

Convection Equation: $\phi_t + v.\nabla\phi = 0$

Regularized Equations

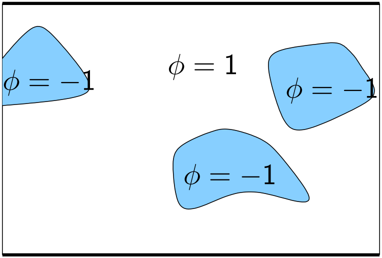


Momentum Equation

$$\int_\Omega \Big\{ (v_t + (v.\nabla)v, w) - (p, div(w)) + \nu(D(v), D(w)) + \gamma\left(\epsilon\Delta\phi - (1/\epsilon)F'(\phi), \nabla\phi.w\right) \Big\} = \int_\Omega f.w.$$

Convection Equation: $\phi_t + v.\nabla\phi = \epsilon\Delta\phi - (1/\epsilon)F'(\phi)$

Regularized Equations

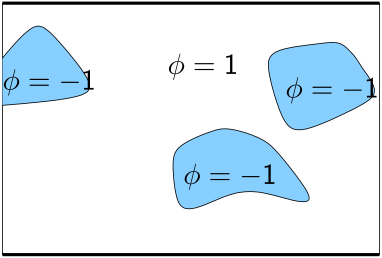


Momentum Equation

$$\int_\Omega \Big\{ (v_t + (v.\nabla)v, w) - (p, div(w)) + \nu(D(v), D(w)) \\ + \gamma\left(\phi_t + v.\nabla\phi, \nabla\phi.w\right) \Big\} = \int_\Omega f.w.$$

Convection Equation: $\phi_t + v.\nabla\phi = \epsilon\Delta\phi - (1/\epsilon)F'(\phi)$

Regularized Equations



Momentum Equation

$$\int_\Omega \Big\{ (v_t + (v.\nabla)v, w) - (p, div(w)) + \nu(D(v), D(w)) \\ + \gamma\left(\phi_t + v.\nabla\phi, \nabla\phi.w\right)\Big\} \quad = \quad \int_\Omega f.w.$$

$$\int_\Omega (\phi_t + v.\nabla\phi)\psi + \epsilon\nabla\phi.\nabla\psi + (1/\epsilon)F'(\phi)\psi = 0$$

Regularized Equations

Energy Estimate

- Set $w = v$ in the momentum equation
- and $\psi = \phi_t$ in the phase equation

$$\frac{d}{dt}\int_\Omega \left\{(|v|^2/2) \quad + \quad \gamma\left((\epsilon/2)|\nabla\phi|^2 + (1/\epsilon)F(\phi)\right)\right\}$$

$$+ \quad \int_\Omega \gamma(\phi_t + v.\nabla\phi)^2 + \nu|D(v)|^2 = \int_\Omega (f, v).$$

Formal Asymptotics

- $\displaystyle\int_\Omega (\epsilon/2)|\nabla\phi|^2 + (1/\epsilon)F(\phi) \simeq (4/3)A$
- $\displaystyle\int_\Omega (\phi_t + v.\nabla\phi)^2 = \int_\Omega \left(\epsilon\Delta\phi - (1/\epsilon)F'(\phi)\right)^2 \simeq \int_\Omega (4\epsilon/3)|H|^2$

Maximum Principle: $|\phi(t, x)| \leq 1$

Regularized Equations

Energy Estimate

- Set $w = v$ in the momentum equation
- and $\psi = \phi_t$ in the phase equation

$$\frac{d}{dt}\int_\Omega \Big\{(|v|^2/2) \quad + \quad \gamma\left((\epsilon/2)|\nabla\phi|^2 + (1/\epsilon)F(\phi)\right)\Big\}$$
$$+ \quad \int_\Omega \gamma(\phi_t + v.\nabla\phi)^2 + \nu|D(v)|^2 = \int_\Omega (f, v).$$

Theorem: (njw) *"Numerical approximations using*

- *DG approximations of the regularized momentum equations*
- *CG approximations of the regularized convection equation*

converge"

Liquid Crystals: The Ericksen-Leslie equations for nematic liquid crystals have this structure.

Extensions

Unbounded Operators: $U_h \subset W \hookrightarrow U \hookrightarrow\!\!\!\!\rightarrow H \hookrightarrow W'$

- $a(u,u) \geq c\|u\|_U^p$
- $|a(u,v)| \leq C\|u\|_U\|v\|_W$
- $\{\|F_h\|_{L^q[0,T;W_h']}\}_{h>0}$
- Assume $P^n : H \to U_h^n$ satisfies $\|P_h u\|_W \leq C\|u\|_W$

Then DG solutions are compact into $L^p[0,T;H] \cap L^r[0,T;W']$ for $1 \leq r < \infty$.

Extensions

Unbounded Operators: $U_h \subset W \hookrightarrow U \hookrightarrow\!\!\!\rightarrow H \hookrightarrow W'$

- $a(u,u) \geq c\|u\|_U^p$
- $|a(u,v)| \leq C\|u\|_U \|v\|_W$
- $\{\|F_h\|_{L^q[0,T;W_h']}\}_{h>0}$
- Assume $P^n : H \to U_h^n$ satisfies $\|P_h u\|_W \leq C\|u\|_W$

Then DG solutions are compact into $L^p[0,T;H] \cap L^r[0,T;W']$ for $1 \leq r < \infty$.

Example: Oldroyd-B Fluid: $T_e \in L^\infty[0,T;L^1(\Omega)]$

$$\int_\Omega (\rho \dot{v}, w) + \mu(D(v), D(w)) = \int_\Omega (\rho f, w) - (T_e, \nabla w)$$

Then $w \mapsto (T_e, \nabla w) \in L^1[0,T;W_0^{1,\infty}(\Omega)']$

$$U_h \subset W_0^{1,\infty}(\Omega) \subset H_0^1(\Omega) \hookrightarrow\!\!\!\rightarrow L^2(\Omega) \hookrightarrow W_0^{1,\infty}(\Omega)'.$$

Extensions

Unbounded Operators: $U_h \subset W \hookrightarrow U \hookrightarrow\!\!\!\!\rightarrow H \hookrightarrow W'$

- $a(u, u) \geq c\|u\|_U^p$
- $|a(u, v)| \leq C\|u\|_U\|v\|_W$
- $\{\|F_h\|_{L^q[0,T;W_h']}\}_{h>0}$
- Assume $P^n : H \to U_h^n$ satisfies $\|P_h u\|_W \leq C\|u\|_W$

Then DG solutions are compact into $L^p[0, T; H] \cap L^r[0, T; W']$ for $1 \leq r < \infty$.

Adaptive Meshing:

- $\{U_h^n\}_{n=1}^N \subset U$
- Assume $P^n : H \to U_h^n$ satisfies $\|u - P_h^n u\|_H \leq Ch\|u\|_U$
- h/τ is bounded

Then DG solutions are compact into $L^p[0, T; H]$