PDEs, modeling & simulation

Achim Schroll

PDEs in Science

- potential theory

$$-\Delta\phi = \rho \quad \rightsquigarrow \quad F = m\nabla\phi$$

- heat transfer

$$T_t + u \cdot \nabla T - \frac{1}{Pe}\Delta T = s$$

- fluid flow

$$u_t + u\nabla u + \nabla p - \frac{1}{Re}\Delta u = f$$
$$\nabla \cdot u = 0$$

- continuum / quantum mechanics

$$u_t + \nabla \cdot F(u) = s \quad , \quad i\hbar\psi_t = \left[\frac{-\hbar^2}{2\mu}\Delta + V\right]\psi$$

vector calculus

$$\nabla = (\partial_{x_1}, \partial_{x_2}, \dots \partial_{x_n})^T$$

$$\nabla f = \mathrm{grad} f$$

$$\Delta f = \nabla \cdot \nabla f = \langle \nabla, \nabla f \rangle = \nabla^T \nabla f = \nabla^2 f$$

$$\nabla \cdot \vec{u} = \langle \nabla, \vec{u} \rangle = \nabla^T \vec{u} = \mathrm{div} \vec{u}$$

$$\nabla \times \vec{u} = \mathrm{rot} \vec{u}$$

vector calculus

product rule

$$\nabla \cdot (g\vec{f}) = \nabla g \cdot \vec{f} + g(\nabla \cdot \vec{f})$$

div–theorem (Gauss's theorem, fundamental theorem of calculus)

$$\int_\Omega \nabla \cdot \vec{f} \,\mathrm{d}x = \int_{\partial\Omega} \vec{f} \cdot \vec{n} \,\mathrm{d}S$$

Green's first identity (partial integration)

$$\int_\Omega g \Delta\phi \,\mathrm{d}x = \int_{\partial\Omega} g \nabla\phi \cdot \vec{n} \,\mathrm{d}S - \int_\Omega \nabla g \cdot \nabla\phi \,\mathrm{d}x$$

classification of linear, second order PDEs

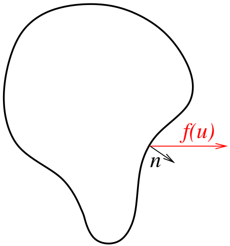
$$Au_{tt} + 2Bu_{tx} + Cu_{xx} + \mathrm{l.o.t.} = 0$$

$$\begin{cases} B^2 - AC < 0 & \text{elliptic} \\ B^2 - AC = 0 & \text{parabolic} \\ B^2 - AC > 0 & \text{hyperbolic} \end{cases}$$

prototypes:

$$\begin{cases} \pm\Delta u = f & \text{Poisson eqn, elliptic} \\ u_t = \nabla \cdot (d\nabla u) & \text{heat eqn, parabolic} \\ u_{tt} = c^2 u_{xx} & \text{wave eqn, hyperbolic} \end{cases}$$

conservation laws



$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega u(t,x)\,\mathrm{d}x + \int_{\partial\Omega} f(u(t,x))\cdot n\,\mathrm{d}S = 0$$

divergence theorem: $\displaystyle\int_{\partial\Omega} f\cdot n\,\mathrm{d}S = \int_\Omega \nabla\cdot f\,\mathrm{d}x$

$$u_t + \nabla\cdot f(u) = 0$$

diffusion

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega u(t,x)\,\mathrm{d}x + \int_{\partial\Omega} f(u(t,x))\cdot n\,\mathrm{d}S = 0$$

Fick's first law (1855): $f(u) = -D\nabla u$

divergence theorem

$$\int_\Omega u_t(t,x) - \nabla\cdot(D\nabla u)\,\mathrm{d}x = 0$$

diffusion / heat equation

$$u_t = \nabla\cdot(D\nabla u)\ , \quad x\in\Omega\ , \quad t>0$$

the Poisson equation

$$\begin{cases} -\Delta u = f & x \in \Omega \\ u(x) = u_0(x) & x \in \partial\Omega \end{cases}$$

variational formulation

$$-\int_\Omega \Delta u v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x$$

Green's first identity

$$\int_\Omega v \Delta w \,\mathrm{d}x = \int_{\partial\Omega} v \frac{\partial w}{\partial n} \,\mathrm{d}S - \int_\Omega \nabla v \cdot \nabla w \,\mathrm{d}x$$

test function $v = 0$ on $\partial\Omega \rightsquigarrow \nabla$ is anti–symmetric:

$$\int_\Omega v \nabla^2 w \,\mathrm{d}x = -\int_\Omega \nabla v \cdot \nabla w \,\mathrm{d}x$$

the Poisson equation

$$-\int_\Omega \nabla \cdot \nabla u v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x$$

weak, variational formulation

$$\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x \ , \quad \forall v \in \widehat{V}$$

solution space

$$V = \{u \in H^1(\Omega) : u = u_0 \text{ on } \partial\Omega\}$$

test space

$$\widehat{V} = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\}$$

Hilbert (Sobolev) spaces

$$(f,g)_{L^2} = \int_\Omega f(x)g(x)\,\mathrm{d}x \ , \quad \|f\|^2_{L^2} = (f,f)_{L^2} = \int_\Omega f(x)^2\,\mathrm{d}x$$

$$L^2(\Omega) = \{f : \|f\|_{L^2} < \infty\}$$

$$(f,g)_{H^1} = \int_\Omega fg + \nabla f \cdot \nabla g\,\mathrm{d}x \ , \quad \|f\|^2_{H^1} = (f,f)_{H^1} = \|f\|^2_{L^2} + \|\nabla f\|^2_{L^2}$$

$$H^1(\Omega) = \{f \in L^2(\Omega) : \nabla f \in L^2(\Omega)\}$$

Hilbert spaces are complete!

weak derivatives in L^2

for $w \in C^1(\Omega)$ recall

$$\int_\Omega \nabla w(x)\phi(x)\,\mathrm{d}x = -\int_\Omega w(x)\nabla\phi(x)\,\mathrm{d}x\ ,\quad \forall\phi \in C_0^\infty(\Omega) \quad (1)$$

for $w \in L^2(\Omega)$ define the weak gradient by (1).

Galerkin formulation / method

find $u \in V$ such that

$$\underbrace{\int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x}_{a(u,v)} = \underbrace{\int_\Omega fv \, \mathrm{d}x}_{l(v)} \ , \quad \forall v \in \widehat{V}$$

Galerkin's method

Find $u_\Delta \in V_\Delta \subset V$ such that

$$a(u_\Delta, v) = l(v) \ , \quad \forall v \in \widehat{V}_\Delta \subset \widehat{V} \ ,$$

where $\dim\,(V_\Delta) = \dim\,(\widehat{V}_\Delta) < \infty$.

Galerkin method

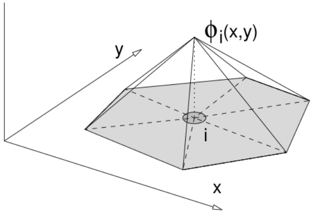
Choose a basis $\{\phi_j\}_{j=1}^{n}$ for V_Δ and $\{\varphi_j\}_{j=1}^{n}$ for $\widehat{V}_\Delta$

$$
\begin{aligned}
u_\Delta &= \textstyle\sum_j \xi_j \phi_j(x) \\
a(\textstyle\sum_j \xi_j \phi_j, v) &= l(v) \ , \quad \forall v \in \widehat{V}_\Delta \\
\textstyle\sum_j a(\phi_j, \varphi_i)\xi_j &= l(\varphi_i) \ , \quad i = 1, 2, \dots, n
\end{aligned}
$$

$$A \cdot \xi = b$$

A is symmetric, regular and positive definite.

Finite Elements



triangulation $\Omega_\Delta = \cup \Delta_k \subset \Omega$,

h_k longest side of Δ_k, $h = \max_k h_k$

interior vertices p_i, pyramid functions ϕ_j: $\phi_j(p_i) = \delta_{ij}$

$$V_\Delta = \text{span }\{\phi_1, \phi_2, \ldots, \phi_N\} \subset H^1(\Omega)$$

$$v \in V_\Delta\colon\ v(x,y) = \sum_{j=1}^{N} v(p_j)\phi_j(x,y)$$

FE Poisson

$$
\begin{aligned}
u_\Delta &= \textstyle\sum_j \xi_j \phi_j(x) \\
\int_{\Omega_\Delta} \nabla u_\Delta \cdot \nabla v \, \mathrm{d}x &= \int_{\Omega_\Delta} f v \, \mathrm{d}x \ , \quad \forall v \in \widehat{V}_\Delta \\
A\xi &= b \\
a_{ij} = a(\phi_j, \phi_i) &= \int_{\Omega_\Delta} \nabla \phi_j \cdot \nabla \phi_i \, \mathrm{d}x \\
b_i = l(\phi_i) &= \int_{\Omega_\Delta} f \phi_i \, \mathrm{d}x
\end{aligned}
$$

automated finite elements: FEniCS

$$\underbrace{\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x}_{a(u,v)} = \underbrace{\int_\Omega f v \,\mathrm{d}x}_{l(v)} \ , \quad \forall v \in \widehat{V}$$

```
a = inner(grad(u), grad(v))*dx
l = f*v*dx
solve(a == l, u, bc)
```

automated finite elements: FEniCS

$$-\Delta u = f \ , \quad u(0,y) = uD \ , \quad \partial u / \partial n = g \ \text{ on } \ \Gamma$$

$$\int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x = \int_\Omega fv \, \mathrm{d}x + \int_\Gamma gv \, \mathrm{d}S \ , \quad \forall v \in \widehat{V}$$

```
bc = DirichletBC(V, uD, "near(x[0],0)")
a = inner(grad(u), grad(v))*dx
l = f*v*dx + g*v*ds

solve(a == l, u, bc)
```

the trace operator

Lemma 1: $C^1(\bar{\Omega})$ is dense in $H^1(\Omega)$.

Definition: Let $\Gamma \subset \partial\Omega$.

$$\begin{aligned} \mathrm{Tr}\colon\ H^1(\Omega) &\rightarrow L^2(\Gamma) \\ u &\mapsto u|_\Gamma \\ u|_\Gamma &:= \lim_{n\to\infty} u_n|_\Gamma \ , \quad u_n \in C^1(\bar{\Omega}) \end{aligned}$$

Lemma 2: $\|u\|_{L^2(\Gamma)} \leq C\|u\|_{H^1(\Omega)}$

Corrolary: By Lemma 2, the trace is a unique extension of boundary values in $C^1(\bar{\Omega})$.

elliptic PDEs

$$
\begin{aligned}
-\Delta u &= f \ , \quad x \in \Omega \\
\partial u / \partial n &= 0 \ , \quad x \in \partial\Omega \ , \quad \int_\Omega u \,\mathrm{d}x = 0
\end{aligned}
$$

variational formulation: $-\int_\Omega \Delta u v \,\mathrm{d}x = \int_\Omega f v \,\mathrm{d}x$

Green's identity: $-\int_{\partial\Omega} v \frac{\partial u}{\partial n} \,\mathrm{d}x + \underbrace{\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x}_{a(u,v)} = \underbrace{\int_\Omega f v \,\mathrm{d}x,}_{l(v)}$

weak formulation: $\quad a(u,v) = l(v) \ , \quad \forall v \in H^1(\Omega)$

Galerkin weak formulation

Find $u \in V$ such that $a(u, v) = l(v)$, $\forall v \in V$

where V is a Hilbert space, $l : V \mapsto \mathbb{R}$ is linear and $a : V \times V \mapsto \mathbb{R}$ is bi–linear.

Assumptions:

- V–ellipticity: $\exists k_1 > 0$ s.t. $a(v, v) \geq k_1 \|v\|_V^2$
- continuity:

  $\exists k_2$ s.t. $|a(v, w)| \leq k_2 \|v\|_V \|w\|_V$

  $\exists k_3$ s.t. $|l(v)| \leq k_3 \|v\|_V$
- and often: symmetry $a(u, v) = a(v, u)$

weak solutions

Lax–Milgram theorem (1954): Under these assumptions, the variational problem has a unique solution $u \in V$

$$\|u\|_V \leq k_3/k_1 \ .$$

Conclusion: The Poisson equation with Neumann boundary conditions has a unique, weak solution $u \in H^1(\Omega)$, $\int_\Omega u \,\mathrm{d}x = 0$ satisfying the bound

$$\|u\|_{H^1} \leq (1 + C)\|f\|_{L^2} \ .$$

tools

Cauchy–Schwarz inequality:

$$|(u, v)| \leq \|u\| \|v\|$$

Poincaré inequality:

If either $v \in H^1(\Omega)$ and $\int_\Omega v \, \mathrm{d}x = 0$, or $v \in H_0^1(\Omega)$

$$\|v\|_{L^2} \leq C \|\nabla v\|_{L^2}$$

by Poincaré, Poisson is H^1–elliptic ...

analysis

$a(u,v) = l(v)$, $\forall v \in V$, (bi–)linear, V–elliptic, and continous

inner product: $a(\cdot,\cdot)$

(energy)–norm $\|v\|_a := \sqrt{a(v,v)}$

norm equivalence: $k_1\|v\|_V^2 \leq a(v,v) \leq k_2\|v\|_V^2$

Galerkin orthogonality: $a(u-u_\Delta, v) = 0$, $\forall v \in V_\Delta$

best approximation: $\|u-u_\Delta\|_a \leq \|u-v\|_a$, $\forall v \in V_\Delta$

Céa–Lemma (error estimate in the V–norm):

$$\|u-u_\Delta\|_V \leq \sqrt{k_2/k_1}\,\|u-v\|_V \quad , \quad \forall v \in V_\Delta \quad .$$

FE analysis

consider Poisson

$$\begin{aligned} -\Delta u &= f \ , \quad x \in \Omega \subset \mathbb{R}^n \\ u &= 0 \ , \quad x \in \partial\Omega \end{aligned}$$

$\Omega \subset \mathbb{R}^n$ convex, smoothly bounded and $f \in L^2(\Omega)$

$$a(u,v) = \int_\Omega \nabla u \cdot \nabla v \mathrm{d}x = \int_\Omega f v \mathrm{d}x = l(v) \ , \quad \forall v \in H_0^1(\Omega)$$

by Lax–Milgram, there is a unique solution $u \in H_0^1(\Omega)$.

In fact $u \in H^2(\Omega) \cap H_0^1(\Omega)$ and $\|u\|_{H^2} \leq (1 + C)\|f\|_{L^2}$

FE analysis

recall piecewise linear interpolation $|f(t) - p_1(t)| \leq Ch^2 \|f''\|_\infty$

analogous:

$$\begin{aligned} I_h v(x) &= \sum_j v(p_j)\phi_j(x) \in V_\Delta \\ \|v - I_h v\|_{L^2} &\leq Ch^2 \|v\|_{H^2} \\ \|\nabla v - \nabla I_h v\|_{L^2} &\leq Ch \|v\|_{H^2} \end{aligned}$$

Theorem 1:

$$\|\nabla u - \nabla u_\Delta\|_{L^2} \leq \|\nabla u - \nabla(I_h u)\|_{L^2} \leq Ch\|u\|_{H^2}$$

FE analysis

dual problem

$$\begin{aligned} -\Delta w &= u - u_\Delta = e \ , \quad x \in \Omega \\ w &= 0 \ , \quad x \in \partial\Omega \end{aligned}$$

weak form:

$$a(v, w) = l(v) = \int_\Omega e(x)v(x)\mathrm{d}x \ , \quad \forall v \in H_0^1(\Omega)$$

pick $v = e$ and find $\|e\|_{L^2}^2 \leq \|\nabla e\|_{L^2} Ch \|w\|_{H^2}$

in fact $w \in H^2$ and $\|w\|_{H^2} \leq C\|e\|_{L^2}$

Theorem 2:

$$\|e\|_{L^2} \leq Ch\|\nabla u - \nabla u_\Delta\|_{L^2} = Ch^2\|u\|_{H^2}$$

the FE system

$$-(p(x)u'(x))' + r(x)u(x) = f(x) \;\; , \quad x \in (a,b)$$

$$u(a) = A \;\; , \quad u(b) = B$$

$$p(x) \geq c_0 > 0 \;\; , \quad r(x) \geq 0$$

weak formulation

$$\underbrace{\int_a^b pu'v' + ruv \,\mathrm{d}x}_{a(u,v)} = \underbrace{\int_a^b fv \,\mathrm{d}x}_{l(v)}$$

FE ansatz

$$u_\Delta(x) = A\phi_0(x) + \sum_{j=1}^{N-1} u_j\phi_j(x) + B\phi_N(x)$$

the FE system

$$\sum_{j=1}^{N} a(\phi_j, \phi_i) u_j = l(\phi_i) - a(\phi_0, \phi_i) A - a(\phi_N, \phi_i) B$$

$$a(\phi_j, \phi_i) = \int_a^b p \phi_j' \phi_i' + r \phi_j \phi_i \,\mathrm{d}x \;, \quad l(\phi_i) = \int_a^b f \phi_i \,\mathrm{d}x$$

$$\frac{1}{h^2} \begin{pmatrix} p_{1/2} + p_{3/2} & -p_{3/2} & \\ -p_{i-1/2} & p_{i-1/2} + p_{i+1/2} & -p_{i+1/2} \\ & -p_{N-3/2} & p_{N-3/2} + p_{N-1/2} \end{pmatrix} \begin{pmatrix} u_1 \\ u_i \\ u_{N-1} \end{pmatrix} +$$

$$+ \begin{pmatrix} r_1 u_1 \\ r_i u_i \\ r_{N-1} u_{N-1} \end{pmatrix} = \begin{pmatrix} f_1 + p_{1/2} A / h^2 \\ f_i \\ f_{N-1} + p_{N-1/2} B / h^2 \end{pmatrix}$$

Condition number

$$\kappa(A) = \|A\| \cdot \|A^{-1}\|$$

$$\frac{\|\delta x\|}{\|x\|} \leq \kappa(A)\frac{\|\delta b\|}{\|b\|} \quad , \quad \frac{\|\delta x\|}{\|x\|} \lesssim \kappa(A)\frac{\|\delta A\|}{\|A\|}$$

When solving a linear system $Ax = b$,
a loss of $k = \log_{10} \kappa(A)$ significant digits may be expected.

Dirichlet, Neumann and Robin conditions

$$
\begin{aligned}
-\Delta u &= f \text{ in } \Omega \\
u &= u_0 \text{ on } \Gamma_D \\
\nabla u \cdot n &= g \text{ on } \Gamma_N \\
\nabla u \cdot n &= p(q-u) \text{ on } \Gamma_R
\end{aligned}
$$

$$
\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x - \int_{\partial\Omega} \nabla u \cdot n v \,\mathrm{d}S = \int_\Omega f v \,\mathrm{d}x \quad , \quad v = 0 \text{ on } \Gamma_D
$$

$$
\int_\Omega \nabla u \cdot \nabla v \,\mathrm{d}x + \int_{\Gamma_R} p u v \,\mathrm{d}S = \int_\Omega f v \,\mathrm{d}x + \int_{\Gamma_N} g v \,\mathrm{d}S + \int_{\Gamma_R} p q v \,\mathrm{d}S
$$

subdomains

let $\Omega = (0,1)^2$ and $\Omega_0 = (0,1) \times (0,1/2)$

define Ω_0:

```
class Omega0(SubDomain):
  def inside(self, x, on_boundary):
  return x[1] <= 0.5 + DOLFIN_EPS
```

create an instance:

```
subdomain0 = Omega0()
```

mark cells in subdomain:

```
subdomains = MeshFunction('size_t', mesh,
mesh.topology().dim())
subdomain0.mark(subdomains, 0)
```

subdomains

```
# define new measures associated with the subdomains
dx = Measure('dx', domain=mesh,
subdomain_data=subdomains)

# bilinear form:
a = k0*inner(grad(u), grad(v))*dx(0)
  + k1*inner(grad(u), grad(v))*dx(1)
```

nonlinear Poisson

$$-\nabla \cdot (q(u)\nabla u) = 0 \rightsquigarrow \int_\Omega q(u)\nabla u \cdot \nabla v \,\mathrm{d}x = 0 \quad \forall v$$

```
u = Function(V)   !!!
F = inner(q(u)*grad(u), grad(v))*dx

# Newton needs a derivative;
du = TrialFunction(V)
DF = derivative(F, u, du)

# compute solution:
problem = NonlinearVariationalProblem(F, u, bc, DF)
solver = NonlinearVariationalSolver(problem)
solver.solve()
```

nonlinear Poisson

Gâteaux (directional) derivative:

$$
\begin{aligned}
DF(u, \delta u, v) &= \lim_{\epsilon \to 0} \frac{F(u + \epsilon \delta u, v) - F(u, v)}{\epsilon} \\
&= \frac{\mathrm{d}}{\mathrm{d}\epsilon} F(u + \epsilon \delta u, v) \bigg|_{\epsilon = 0}
\end{aligned}
$$

Example: $F(u, v) = \int_\Omega q(u) \nabla u \cdot \nabla v \,\mathrm{d}x$

concepts of error quantification

$$Ax = b \ , \qquad A_h x_h = b_h$$

approximation error: $e = x - x_h$
truncation error: $\tau = A - hx - b_h = A_h e$
residual: $\rho = b - Ax_h = Ae$

a–priori analysis:

$$e = A_h^{-1}\tau \ , \quad \|e\| \leq \|A_h^{-1}\|\|\tau\|$$

a–posteriori analysis:

$$e = A^{-1}\rho \ , \quad \|e\| \leq \|A^{-1}\|\|\rho\|$$

concepts of error quantification

duality based analysis:

linear functional: $J : \mathbb{R}^n \to \mathbb{C}$, $x \mapsto J(x) =< x, j >= j^* x$

dual problem:

$$A^* z = j$$

evaluation:

$$J(x) =< x, A^* z >=< Ax, z >=< b, z >$$

$$J(x) - J(x_h) = J(e) =< Ae, z >=< \rho, z >$$

goal oriented adaptivity

$$
\begin{aligned}
-\Delta u &= f \quad \text{in } \Omega \\
u &= 0 \quad \text{on } \Gamma_D \\
\nabla u \cdot n &= g \quad \text{on } \Gamma_N
\end{aligned}
$$

$$\int_\Omega \nabla u \cdot \nabla v \, \mathrm{d}x = \int_\Omega fv \, \mathrm{d}x + \int_{\Gamma_N} gv \, \mathrm{d}S$$

goal: $|M(u) - M(u_\Delta)| \leq Tol$

goal oriented adaptivity

$$
\begin{aligned}
a(u, v) &= l(v) \ , \quad \forall v \in \widehat{V} \\
a(u_\Delta, v) &= l(v) \ , \quad \forall v \in \widehat{V}_\Delta
\end{aligned}
$$

adaptive problem: find V_Δ and u_Δ s.t. $|M(u) - M(u_\Delta)| \leq Tol$

dual problem: find $w \in \widehat{V}$ s.t. $a(v, w) = M(v), \forall v \in V$

$$M(u) - M(u_\Delta) = a(u, w) - a(u_\Delta, w) = l(w) - a(u_\Delta, w) = r(w)$$

compute w and evaluate the dual residual $r(w)$

C. Johnson (1990), R. Rannacher (1995), . . .

adaptivity in FEniCS

```
a = inner(grad(u), grad(v))*dx
l = f*v*dx + g*v*ds
solve(a == l, u, bc, tol=1e-5, M=u*dx)
```

THE WILKINSON PRIZE FOR NUMERICAL SOFTWARE 2015

diffusion

conservation of mass:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega u(t,x)\,\mathrm{d}x + \int_{\partial\Omega} f(u)n\,\mathrm{d}S = 0$$

Fick's first law (1855): $f(u) = -D\nabla u$

divergence theorem

$$\int_\Omega u_t(t,x) - \nabla\cdot(D\nabla u)\,\mathrm{d}x = 0$$

diffusion / heat equation

$$u_t = \nabla\cdot(D\nabla u)\ , \quad x\in\Omega\ , \quad t>0$$

diffusion

$$u_t = \Delta u + f$$

implicit time stepping

$$\frac{u^k - u^{k-1}}{\Delta t} = \Delta u^k + f^k$$

weak variational form

$$\int_\Omega u^k v + \Delta t \nabla u^k \cdot \nabla v \, \mathrm{d}x = \int_\Omega \left(u^{k-1} + \Delta t f^k \right) v \, \mathrm{d}x \ , \quad \forall v \in H_0^1(\Omega)$$

diffusion

naive code:

```
while t <= T:
      a = u*v*dx + dt*inner(grad(u), grad(v))*dx
      l = (u_1 + dt*f)*v*dx
      solve(a == l, u, bc)
```

diffusion

naive code:

```
while t <= T:
      a = u*v*dx + dt*inner(grad(u), grad(v))*dx
      l = (u_1 + dt*f)*v*dx
      solve(a == l, u, bc)
```

pre–assembled:

```
A = assemble(a)
while t <= T:
      b = assemble(l, tensor=b)
      bc.apply(A, b)
      solve(A, u.vector(), b)
```

time stepping

$$y' = f(y) \ , \quad y(0) = y_0$$

explicit Euler

$$\frac{y^{k+1} - y^k}{\Delta t} = f(u^k)$$

implicit Euler

$$\frac{y^{k+1} - y^k}{\Delta t} = f(u^{k+1})$$

trapezoidal method (leap–frog)

$$\frac{y^{k+1} - y^k}{\Delta t} = \frac{1}{2}\left(f(u^{k+1}) + f(u^k)\right)$$

time stepping and stability

test equation: $y' = \lambda y \;\; , \quad y(0) = 1 \;\; , \quad y(t) = \exp(\lambda t)$

time stepping: $y^{k+1} = y^k + \Delta t b_1 \lambda y^{k+1} + \Delta t b_0 \lambda y^k$

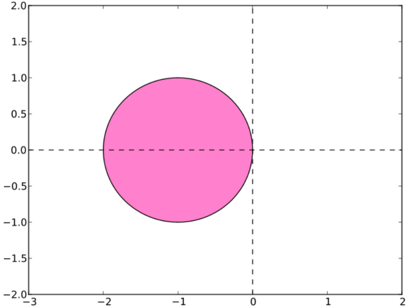
$$y^{k+1} = R(\Delta t \lambda) y^k \;\; , \quad R(z) = \frac{1 + b_0 z}{1 - b_1 z}$$

stability condition: $|R(z)| \leq 1$ for all $z \in \mathbb{C}^-$.

time stepping and stability

explicit Euler: $b_0 = 1$, $b_1 = 0$, $R(z) = 1 + z$

stability area: $S = \{z \in \mathbb{C} : |1 + z| \leq 1\}$

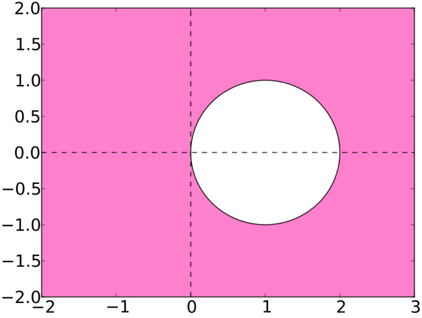


conditional stability: Δt small enough!

time stepping and stability

implicit Euler: $b_0 = 0$, $b_1 = 1$, $R(z) = \frac{1}{1-z}$

stability area: $S = \{z \in \mathbb{C} : 1 \leq |1 - z|\}$

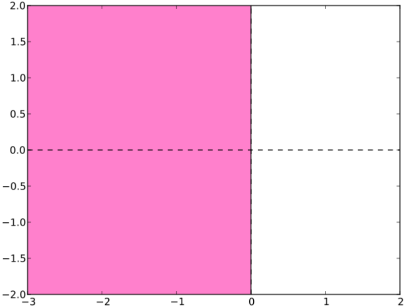


A–stability: $\mathbb{C}^- \subset S$

time stepping and stability

trapezoidal method: $b_0 = 1/2$, $b_1 = 1/2$, $R(z) = \frac{1+z/2}{1-z/2}$

stability area: $S = \{z \in \mathbb{C} : |1 + z/2| \leq |1 - z/2|\}$



A–stability: $S = \mathbb{C}^-$

time stepping and stability

test equation: $y' = \lambda y \;, \quad y(0) = 1 \;, \quad y(t) = \exp(\lambda t)$

if $\mathrm{Re}(\lambda) \to -\infty$, then $y(t) = \exp(\lambda t) \to 0$.

discrete: $y^{k+1} = R(\Delta t \lambda) y^k$

An A–stable method with $\lim_{|z|\to\infty} R(z) = 0$ is called L–stable.

Remark: If $R(z) = \frac{P(z)}{Q(z)}$ and $\lim_{|z|\to\infty} R(z) < \infty$, then

$$\deg(P) \leq \deg(Q) \text{ and}$$

$$\lim_{x\to-\infty} R(x) = \lim_{x\to+\infty} R(x) = \lim_{x\to\pm\infty} R(ix) \;, \quad x \in \mathbb{R}$$

.

Remark: implicit Euler is L–stable.

Remark: explicit Euler and trapezoidal method are not.

Remark: any method with "perfect" stability area $S = \mathbb{C}^-$ is not L–stable.

s–stage RK–method

$$k_i = f(t_n + c_i h, y_n + h \sum_{j=1}^{s} a_{ij} k_j)$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i k_i$$

Butcher tableau: $\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$

SDIRK–method

Singly Diagonal Impicit RK–methods:

$$\begin{array}{c|cc} \gamma & \gamma & \\ 1-\gamma & 1-2\gamma & \gamma \\ \hline & 1/2 & 1/2 \end{array}$$

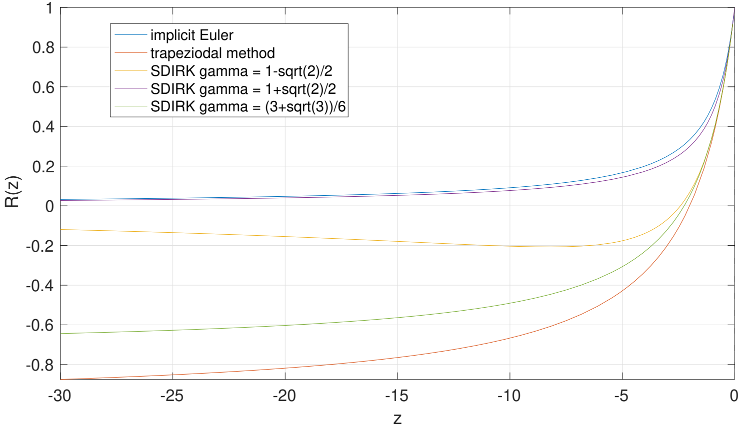
order $p \geq 2$ by construction; order $p = 3$: $\gamma = (3 \pm \sqrt{3})/6$

stability function:

$$R(z) = \frac{1 + z(1-2\gamma) + z^2(1/2 - 2\gamma + \gamma^2)}{(1-\gamma z)^2}$$

SDIRK–method

stability functions along $\mathbb{R}^-$



SDIRK–method

A–stable: $\gamma \geq 1/4$

A–stable & order $p = 3$: $\gamma = (3 + \sqrt{3})/6$

L–stable: $\gamma = (2 \pm \sqrt{2})/2$

L–stable, monotone & order $p = 2$: $\gamma = (2 + \sqrt{2})/2$

wave equation as a system

$$u_{tt} = c^2 \Delta u \ , \quad \begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} v \\ c^2 \Delta u \end{pmatrix}$$

```
W = VectorFunctionSpace(mesh, "CG", 1)
(u,v) = TrialFunctions(W)
w = Function(W)
(u,v) = w.split()
```

Navier–Stokes

conservation of mass:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho(t,x)\,\mathrm{d}x + \int_{\partial\Omega} f(\rho) n \,\mathrm{d}S = 0$$

convective transport $f(\rho) = v\rho$, divergence theorem ...

$$\rho_t + \nabla \cdot (\rho v) = 0$$

incompressible flow: $\rho \equiv 1 \rightsquigarrow \nabla \cdot v = 0$

Navier–Stokes

conservation of momentum:

$$\rho(v_t + v \cdot \nabla v) = -\nabla p + \nu \Delta v + f$$

incompressible Navier–Stokes (1822)

$$\begin{aligned} v_t + v \cdot \nabla v + \nabla p &= \nu \Delta v + f \\ \nabla \cdot v &= 0 \end{aligned}$$

remark: $v \cdot \nabla v = v \cdot (\nabla v) = (v \cdot \nabla) v$

Navier–Stokes

$$\frac{v^n - v^{n-1}}{\Delta t} + (v^{n-1} \cdot \nabla) v^{n-1} = -\nabla p^n + \nu \Delta v^{n-1} + f^{n-1}$$

Chorin's projection method (1968):

1. find a tentative velocity v^*

$$\frac{v^* - v^{n-1}}{\Delta t} + (v^{n-1} \cdot \nabla) v^{n-1} = \nu \Delta v^{n-1} + f^{n-1}$$

   thus, $v^n - v^* = -\Delta t \nabla p^n$ and $\nabla \cdot v^n = \nabla \cdot v^* - \Delta t \Delta p^n = 0$

2. compute the pressure

$$\Delta t \Delta p^n = \nabla \cdot v^*$$

3. update the velocity

$$v^n = v^* - \Delta t \nabla p^n$$

Helmholtz–Hodge decoposition

Helmholtz decomposition (1858): Ω simply connected, $u : \Omega \to \mathbb{R}^n$

$$u = u_{div} + u_{rot} \ , \quad \nabla \cdot u_{div} = 0 \ , \quad \nabla \times u_{rot} = 0 \ .$$

A conservative field $v = \nabla\phi$ is irrotational $\nabla \times \nabla\phi = 0$.
A irrotational field is conservative $u_{rot} = \nabla\phi$.
A divergence–free field has a vector potential $u_{div} = \nabla \times A$.

$$-\Delta\phi = \nabla \cdot u \ , \quad u_{rot} = -\nabla\phi \ , \quad u_{div} = u + \nabla\phi$$

scalar / vector potential: $u = -\nabla\phi + \nabla \times A$

Navier–Stokes

$$\left(\frac{v^n - v^{n-1}}{\Delta t}, \phi\right) + \left(v^{n-1} \cdot \nabla v^{n-1}, \phi\right) + \left(\nabla p^n, \phi\right) + \left(\nu \nabla v^{n-1}, \nabla \phi\right) = \left(f^{n-1}, \phi\right)$$

Chorin in weak form:

1. prediction

$$\left(\frac{v^* - v^{n-1}}{\Delta t}, \phi\right) + \left(v^{n-1} \cdot \nabla v^{n-1}, \phi\right) + \left(\nu \nabla v^*, \nabla \phi\right) = \left(f^{n-1}, \phi\right)$$

2. pressure $\Delta t \left(\nabla p^n, \nabla \psi\right) = -\left(\nabla \cdot v^*, \psi\right)$

3. correction $\left(v^n, \phi\right) = \left(v^*, \phi\right) - \Delta t \left(\nabla p^n, \phi\right)$

demos: `NS_Lpipe.py`, `NS_dolfin.py`

Navier–Stokes

$$\rho(v_t + v \cdot \nabla v) + \nabla p = \nu \Delta v + f \quad , \quad \nabla \cdot v = 0$$

$$\Delta u = \nabla \cdot \nabla u = \nabla \cdot \left(\nabla u + (\nabla u)^T \right) \quad , \quad \nabla \cdot u = 0$$

symmetric gradient:

$$\epsilon(u) = \frac{1}{2} \left(\nabla u + (\nabla u)^T \right)$$

Cauchy stress:

$$\sigma(v, p) = 2\nu\epsilon(v) - pI$$

$$\rho(v_t + v \cdot \nabla v) = \nabla \cdot \sigma(v, p) + f \quad , \quad \nabla \cdot v = 0$$

Navier–Stokes

$$\rho\left(\frac{v^n - v^{n-1}}{\Delta t} + v^{n-1}\cdot\nabla v^{n-1}\right) = \nabla\cdot\sigma(v^{n-1/2}, p^{n-1/2}) + f^{n-1/2}$$

Incremental Pressure Correction (1979):

1. tentative velocity v^*

$$\rho\left(\frac{v^* - v^{n-1}}{\Delta t} + v^{n-1}\cdot\nabla v^{n-1}\right) = \nabla\cdot\sigma(v^{n-1/2}, p^{n-3/2}) + f^{n-1/2}$$

   for computing: $v^{n-1/2} = \frac{1}{2}(v^* + v^{n-1})$

2. pressure update

$$-\Delta t \Delta p^{n-1/2} = -\Delta t \Delta p^{n-3/2} - \rho\nabla\cdot v^*$$

3. velocity correction

$$\rho v^n = \rho v^* - \Delta t \nabla(p^{n-1/2} - p^{n-3/2})$$

Navier–Stokes

partial integration

$$-\int_\Omega \nabla \cdot \sigma(v,p)\,\phi\,\mathrm{d}x = \int_\Omega \sigma(v,p) : \epsilon(\phi)\,\mathrm{d}x - \int_{\partial\Omega} \sigma(v,p)\cdot n\,\phi\,\mathrm{d}S$$

tensor scalar product

$$A : B = \sum_i \sum_j a_{ij} b_{ij}$$

Navier–Stokes

tentative velocity in weak form:

$$\frac{\rho}{\Delta t}\left(v^{*} - v^{n-1}, \phi\right) + \rho\left(v^{n-1} \cdot \nabla v^{n-1}, \phi\right)$$
$$+ \Big(\sigma(v^{n-1/2}, p^{n-3/2}) : \epsilon(\phi)\Big) - \Big(\sigma(v^{n-1/2}, p^{n-3/2}) \cdot n, \phi\Big)_{\partial\Omega}$$
$$= \Big(f^{n-1/2}, \phi\Big)$$

free outflow boundary $\nabla v \cdot n = 0$:

$$\sigma(v, p) \cdot n = (2\nu\epsilon(v) - pI) \cdot n = \nu(\nabla v)^{T} \cdot n - pn$$

Dirichlet boundary (non–slip) $\phi = 0$.

Navier–Stokes

IPC weak form:

1. prediction

$$\frac{\rho}{\Delta t}\left(v^* - v^{n-1}, \phi\right) + \left(v^{n-1} \cdot \nabla v^{n-1}, \phi\right)$$
$$+ \left(\sigma(v^{n-1/2}, p^{n-3/2}) : \epsilon(\phi)\right) + \left((p^{n-3/2} - \nu(\nabla v^{n-1/2})^T) \cdot n, \phi\right)_{\partial\Omega}$$
$$= \left(f^{n-1/2}, \phi\right)$$

2. incremental pressure update

$$\Delta t \left(\nabla p^{n-1/2}, \nabla \psi\right) = \Delta t \left(\nabla p^{n-3/2}, \nabla \psi\right) - \rho \left(\nabla \cdot v^*, \psi\right)$$

3. velocity correction

$$\rho\left(v^n, \phi\right) = \rho\left(v^*, \phi\right) - \Delta t \left(\nabla(p^{n-1/2} - p^{n-3/2}), \phi\right)$$

demo: `NS_dolfin_IPC.py`

Navier–Stokes

incompressible flow with heat transfer

$$
\begin{aligned}
v_t + v \cdot \nabla v + \nabla p &= \frac{1}{Re} \Delta v + f \\
\nabla \cdot v &= 0 \\
T_t + v \cdot \nabla T &= \frac{1}{Pe} \Delta T + s
\end{aligned}
$$

Navier–Stokes

Chorin's projection:

1. tentative velocity v^*

$$\frac{v^* - v^{n-1}}{\Delta t} + (V \cdot \nabla) v^{n-1} = \frac{1}{Re} \Delta v^* + f^{n-1}$$

2. pressure $\Delta t \Delta p^n = \nabla \cdot v^*$

3. velocity $v^n = v^* - \Delta t \nabla p^n$

4. temperature update

$$\frac{c^n - c^{n-1}}{\Delta t} + (V \cdot \nabla) c^{n-1} = \frac{1}{Pe} \Delta c^n + s^{n-1}$$

$V = v^{n-1}$ or, alternatively $V = \frac{1}{2}(v^n + v^{n-1})$.

Navier–Stokes

Chorin in weak form:

1. prediction

$$\left(\frac{v^* - v^{n-1}}{\Delta t}, \phi\right) + \left(V \cdot \nabla v^{n-1}, \phi\right) + \left(\frac{1}{Re}\nabla v^*, \nabla\phi\right) = 0$$

2. pressure $\Delta t \left(\nabla p^n, \nabla\psi\right) = -\left(\nabla \cdot v^*, \psi\right)$

3. correction $\left(v^n, \phi\right) = \left(v^*, \phi\right) - \Delta t \left(\nabla p^n, \phi\right)$

4. temperature

$$\left(\frac{c^n - c^{n-1}}{\Delta t}, \psi\right) + \left(V \cdot \nabla c^{n-1}, \psi\right) + \left(\frac{1}{Pe}\nabla c^n, \nabla\psi\right) = 0$$

demo: `NST_dolfin.py`

Navier–Stokes

IPC:

1. tentative velocity v^*

$$\frac{v^* - v^{n-1}}{\Delta t} + v^{n-1} \cdot \nabla v^{n-1} = \nabla \cdot \sigma(v^{n-1/2}, p^{n-3/2}) + f^{n-1/2}$$

2. pressure update

$$-\Delta t \Delta p^{n-1/2} = -\Delta t \Delta p^{n-3/2} - \rho \nabla \cdot v^*$$

3. velocity correction

$$v^n = v^* - \Delta t \nabla (p^{n-1/2} - p^{n-3/2})$$

4. temperature update

$$\frac{c^n - c^{n-1}}{\Delta t} + (V \cdot \nabla) c^{n-1} = \frac{1}{Pe} \Delta c^n + s^{n-1}$$

Navier–Stokes

IPC weak form:

1. prediction

$$
\begin{aligned}
&\tfrac{1}{\Delta t}\left(v^{*} - v^{n-1}, \phi\right) + \left(v^{n-1}\cdot\nabla v^{n-1}, \phi\right)\\
&+ \left(\sigma(v^{n-1/2}, p^{n-3/2}) : \epsilon(\phi)\right) + \left((p^{n-3/2}) - \tfrac{1}{Re}(\nabla v^{n-1/2})^{T}\right)\cdot n, \phi\big)_{\partial\Omega}\\
&= \left(f^{n-1/2}, \phi\right)
\end{aligned}
$$

2. pressure update
$$\Delta t\left(\nabla p^{n-1/2}, \nabla\psi\right) = \Delta t\left(\nabla p^{n-3/2}, \nabla\psi\right) - \rho\left(\nabla\cdot v^{*}, \psi\right)$$

3. velocity correction
$$(v^{n}, \phi) = (v^{*}, \phi) - \Delta t\left(\nabla(p^{n-1/2} - p^{n-3/2}), \phi\right)$$

4. temperature update
$$\left(\frac{c^{n}-c^{n-1}}{\Delta t}, \psi\right) + \left(V\cdot\nabla c^{n-1}, \psi\right) + \left(\tfrac{1}{Pe}\nabla c^{n}, \nabla\psi\right) = 0$$

demo: `NST_dolfin_IPC.py`

Chorin's pressure correction at higher order?
recall trapezoidal rule:

$$\frac{\Delta t}{2}\left(f(0)+f(h)\right)=\int_0^{\Delta t} f(t)\,\mathrm{d}t+\mathcal{O}(\Delta t^3)$$

analogous

$$\frac{\Delta t}{2}\left(f(0)g(\Delta t)+f(\Delta t)g(0)\right)=\int_0^{\Delta t}(fg)(t)\,\mathrm{d}t+\mathcal{O}(\Delta t^3)$$

Navier–Stokes

$$\frac{v^n - v^{n-1}}{\Delta t} + \int_{t_{n-1}}^{t_n} (v \cdot \nabla) v \,\mathrm{d}t + \int_{t_{n-1}}^{t_n} \nabla p \,\mathrm{d}t = \nu \int_{t_{n-1}}^{t_n} \Delta v \,\mathrm{d}t$$

2. order projection method:

1. find a tentative velocity v^*

$$\frac{v^* - v^{n-1}}{\Delta t} + \frac{1}{2}\left(v^* \cdot \nabla v^{n-1} + v^{n-1} \cdot \nabla v^*\right) = \frac{\nu}{2}\Delta(v^* + v^{n-1})$$

thus, $v^n - v^* + \Delta t \nabla p^{n-1/2} = \mathcal{O}(\Delta t^3)$

2. compute the pressure

$$\Delta t \Delta p^{n-1/2} = \nabla \cdot v^*$$

3. update the velocity

$$v^n = v^* - \Delta t \nabla p^{n-1/2}$$

Navier–Stokes

$$\frac{v^n - v^{n-1}}{\Delta t} + \int_{t_{n-1}}^{t_n} (v \cdot \nabla) v \,\mathrm{d}t = \int_{t_{n-1}}^{t_n} \nabla \cdot \sigma(v, p) \,\mathrm{d}t$$

2. order IPC method:

1. find a tentative velocity v^*

   $$\frac{v^* - v^{n-1}}{\Delta t} + \frac{1}{2}\left(v^* \cdot \nabla v^{n-1} + v^{n-1} \cdot \nabla v^*\right) = \nabla \cdot \sigma(v^{n-1/2}, p^{n-3/2})$$

   thus, $v^n - v^* + \Delta t \nabla \left(p^{n-1/2} - p^{n-3/2}\right) = \mathcal{O}(\Delta t^3)$
2. compute the pressure update

   $$\Delta t \Delta \delta p = \nabla \cdot v^* \quad , \quad p^{n-1/2} = p^{n-3/2} + \delta p$$
3. update the velocity

   $$v^n = v^* - \Delta t \nabla \delta p$$

Navier–Stokes

nonlinear heat transfer $T_t + v \cdot \nabla T = \frac{1}{Pe} \nabla \cdot \left((1 + T^2) \nabla T \right)$

$$\left(\frac{c^n - c^{n-1}}{\Delta t}, \psi \right) + \left(V \cdot \nabla c^{n-1}, \psi \right) + \frac{1}{Pe} \left((1 + (c^n)^2) \nabla c^n, \nabla \psi \right) = 0$$

```
F = inner(c-c0, psi)*dx/dt \
  + inner(dot(V, grad(c0)) ,psi)*dx \
  + (1+c**2)*inner(grad(c), grad(psi))*dx/Pe

solve(F == 0, c, bc)
```

demo: `NST_nonlin_dolfin.py`

Lax & Riesz theorems

$$a(u,v) = l(v)\ ,\quad \forall v \in V$$

V Hilbert space, a and l are (bi–)linear, V–elliptic and continuous

Lax–Milgram theorem (1954):

There **is** a unique, bounded solution in V.

Riesz representation theorem (1907):

There is a unique solution $u \in V$ to

$$(u,v)_V = l(v)\ ,\quad \forall v \in V$$

and $\|u\| = \|l\|$.

Lax & Riesz theorems

Remark: $l : V \to \mathbb{R}$, linear i.e. $l \in V^*$. Riesz: $V \leftrightarrow V^*$

Lemma: The variational problem

$$(u, v)_V = l(v) \ , \quad \forall v \in V$$

is equivalent to

$$u = \arg\min_{v \in V} J(v) \ , \quad J(v) = \frac{1}{2}(v, v) - l(v)$$

calibration of diffusive PDE models

Find α in $u_t = \nabla \cdot (\alpha \nabla u)$ s.t. $J(u(\alpha)) = \int_D (\widetilde{u} - u(\alpha))^2 \, \mathrm{d}x = \min$

$$PDE(u, \alpha) = 0 \ , \quad J(u(\alpha)) = \min \iff J_\alpha(u(\alpha)) = 0$$

Landweber algorithm (1951):

1. solve $PDE(u^k, \alpha^k)$ for u^k
2. evaluate $d^k = J_\alpha(u^k(\alpha^k))$
3. update $\alpha^{k+1} = \alpha^k - \Delta\alpha^k d^k$ (steepest descent)

gradients via duals

$$u_t = \nabla \cdot (\alpha \nabla u) \ , \quad \int_\Omega u_t \phi + \alpha \nabla u \cdot \nabla \phi \, \mathrm{d}x = 0$$

$$\mathcal{A}(u_\alpha, \phi) := \int_\Omega u_{\alpha,t} \phi + \alpha \nabla u_\alpha \cdot \nabla \phi \, \mathrm{d}x = - \int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}x$$

$$J = \int_D (\widetilde{u} - u)^2 \, \mathrm{d}x \ , \quad J_\alpha = -2 \int_D (\widetilde{u} - u) u_\alpha \, \mathrm{d}x$$

gradients via duals

$$u_t = \nabla \cdot (\alpha \nabla u) \ , \quad \int_\Omega u_t \phi + \alpha \nabla u \cdot \nabla \phi \, \mathrm{d}x = 0$$

$$\mathcal{A}(u_\alpha, \phi) := \int_\Omega u_{\alpha,t} \phi + \alpha \nabla u_\alpha \cdot \nabla \phi \, \mathrm{d}x = - \int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}x$$

$$J = \int_D (\widetilde{u} - u)^2 \, \mathrm{d}x \ , \quad J_\alpha = -2 \int_D (\widetilde{u} - u) u_\alpha \, \mathrm{d}x$$

$$\mathcal{A}^*(\omega, \phi) = \mathcal{A}(\phi, \omega) = -2 \int_D (\widetilde{u} - u) \phi \, \mathrm{d}x \ , \quad \forall \phi$$

gradients via duals

$$u_t = \nabla \cdot (\alpha \nabla u) \ , \quad \int_\Omega u_t \phi + \alpha \nabla u \cdot \nabla \phi \, \mathrm{d}x = 0$$

$$\mathcal{A}(u_\alpha, \phi) := \int_\Omega u_{\alpha,t} \phi + \alpha \nabla u_\alpha \cdot \nabla \phi \, \mathrm{d}x = -\int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}x$$

$$J = \int_D (\widetilde{u} - u)^2 \, \mathrm{d}x \ , \quad J_\alpha = -2 \int_D (\widetilde{u} - u) u_\alpha \, \mathrm{d}x$$

$$\mathcal{A}^*(\omega, \phi) = \mathcal{A}(\phi, \omega) = -2 \int_D (\widetilde{u} - u) \phi \, \mathrm{d}x \ , \quad \forall \phi$$

$$\mathcal{A}(u_\alpha, \omega) = -2 \int_D (\widetilde{u} - u) u_\alpha \, \mathrm{d}x = J_\alpha$$

gradients via duals

$$u_t = \nabla \cdot (\alpha \nabla u) \ , \quad \int_\Omega u_t \phi + \alpha \nabla u \cdot \nabla \phi \,\mathrm{d}x = 0$$

$$\mathcal{A}(u_\alpha, \omega) := \int_\Omega u_{\alpha,t}\omega + \alpha \nabla u_\alpha \cdot \nabla \omega \,\mathrm{d}x = -\int_\Omega \nabla u \cdot \nabla \omega \,\mathrm{d}x$$

$$J = \int_D (\widetilde{u} - u)^2 \,\mathrm{d}x \ , \quad J_\alpha = -2 \int_D (\widetilde{u} - u) u_\alpha \,\mathrm{d}x$$

$$\mathcal{A}^*(\omega, \phi) = \mathcal{A}(\phi, \omega) = -2 \int_D (\widetilde{u} - u)\phi \,\mathrm{d}x \ , \quad \forall \phi$$

$$\mathcal{A}(u_\alpha, \omega) = -2 \int_D (\widetilde{u} - u) u_\alpha \,\mathrm{d}x = J_\alpha = -\int_\Omega \nabla u \cdot \nabla \omega \,\mathrm{d}x$$

dual problem

$$\mathcal{A}^*(\omega, \phi) = -2 \int_D (\widetilde{u} - u)\phi \, \mathrm{d}x \ , \quad \forall \phi$$

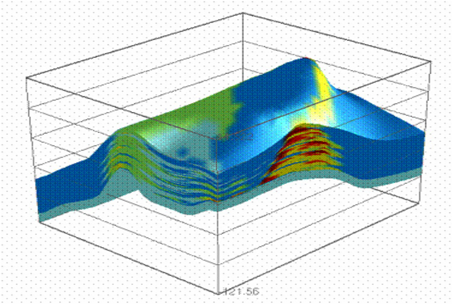
dual problem

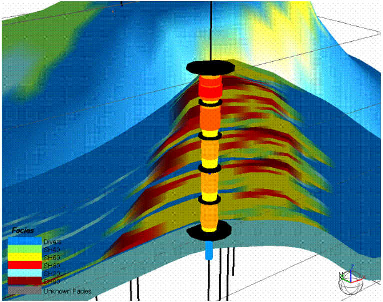
$$\mathcal{A}^*(\omega, \phi) = -2 \int_D (\widetilde{u} - u)\phi \, \mathrm{d}x \;\; , \quad \forall \phi$$

$$\int_\Omega \phi_t \omega + \alpha \nabla \phi \cdot \nabla \omega \, \mathrm{d}x = -2 \int_D (\widetilde{u} - u)\phi \, \mathrm{d}x \;\; , \quad \forall \phi$$

$$-\omega_t = \nabla \cdot (\alpha \nabla \omega) - 2(\widetilde{u} - u)|_D \;\; , \quad t : T \to 0$$

depositional modelling





depositional modelling

$$\begin{pmatrix} A & s \\ -A & 1-s \end{pmatrix} \begin{pmatrix} s \\ h \end{pmatrix}_t = \nabla \cdot \begin{pmatrix} \alpha \, s \nabla h \\ \beta \, (1-s) \nabla h \end{pmatrix}$$

well–output: $J(p) = \frac{1}{|W|} \int_0^T \int_W (\widetilde{u}(t,x) - u(p,t,x))^2 \, dx \, dt$

forward problem:

- mapping: parameter $\rightarrow$ observation
- transport coefficients $\rightarrow$ well–output

calibration, an inverse problem

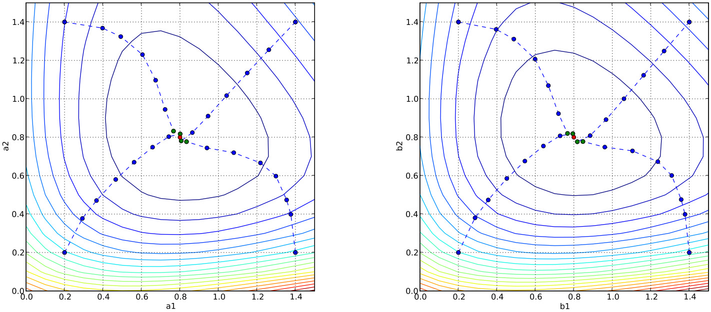
$$\begin{pmatrix} A & s \\ -A & 1-s \end{pmatrix} \begin{pmatrix} s \\ h \end{pmatrix}_t = \nabla \cdot \begin{pmatrix} \alpha \; s \nabla h \\ \beta \; (1-s) \nabla h \end{pmatrix}$$

well–output: $J(p) = \frac{1}{|W|} \int_0^T \int_W (\tilde{u}(t,x) - u(p,t,x))^2 \, dx \, dt$

inverse problem:

- inv. mapping: parameter $\leftarrow$ observation
- transport coefficients $\leftarrow$ well–output

the output functional



the output functional

$$u_t = d\Delta u \ , \quad d > 0$$

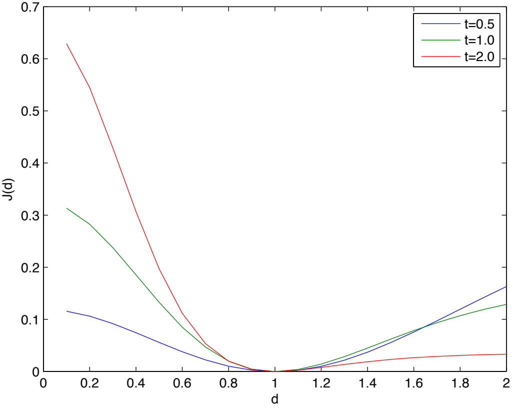
$$K(td, x) = \frac{1}{(4\pi td)^{n/2}} e^{-|x|^2/4td} \ , \quad x \in \mathbb{R}^n$$

$$u(td, x) = \int K(td, x - y) f(y) \, dy \ , \quad u(0, x) = f(x)$$

$$J(d) = \int (u(td, x) - u(t, x))^2 \, \mathrm{d}x$$

$$J(1) = 0 \ , \quad J'(1) = 0 \ , \quad J''(1) = 2t^2 \|\Delta u(t, x)\|^2 > 0$$

the output functional



$$u(t,x,d) = e^{-d^2 t} \sin(\sqrt{d/2}x_1) \cos(\sqrt{d/2}x_2)$$

outlook – automated, adaptive calibration

$$\begin{aligned} u_t &= \nabla \cdot (\alpha \nabla u) + f \\ \int_\Omega u_t \phi + \alpha \nabla u \cdot \nabla \phi \, \mathrm{d}x &= \int_\Omega f \phi \, \mathrm{d}x \ , \quad \forall \phi \\ a(\alpha, u, \phi) &= l(\phi) \ , \quad \forall \phi \end{aligned}$$

misfit functional:

$$J(\alpha, u) = \|\widetilde{u} - u\|^2 + \eta \|\alpha\|^2 \to \min$$

Lagrange functional:

$$L(\alpha, u, \omega) = \underbrace{J(\alpha, u)}_{\to \min} \underbrace{- a(\alpha, u, \omega) + l(\omega)}_{\to 0}$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

primal problem ∂_ω:

$$-a_\omega(\alpha, u, \omega)(\phi) + l_\omega(\omega)(\phi) = 0 \;\;, \quad \forall \phi$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

primal problem ∂_ω:

$$-a_\omega(\alpha, u, \omega)(\phi) + l_\omega(\omega)(\phi) = 0 \quad , \quad \forall \phi$$

$$a(\alpha, u, \phi) = l(\phi) \quad , \quad \forall \phi$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

primal problem ∂_ω:

$$-a_\omega(\alpha, u, \omega)(\phi) + l_\omega(\omega)(\phi) = 0 \ , \quad \forall \phi$$

$$a(\alpha, u, \phi) = l(\phi) \ , \quad \forall \phi$$

$$\int_\Omega u_t \phi + \alpha \nabla u \cdot \nabla \phi \, \mathrm{d}x = \int_\Omega f \phi \, \mathrm{d}x \ , \quad \forall \phi$$

$$u_t = \nabla \cdot (\alpha \nabla u) + f$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

dual problem ∂_u:

$$J_u(\alpha, u)(\psi) - a_u(\alpha, u, \omega)(\psi) = 0 \ , \quad \forall \psi$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

dual problem ∂_u:

$$J_u(\alpha, u)(\psi) - a_u(\alpha, u, \omega)(\psi) = 0 \ , \quad \forall \psi$$

$$a(\alpha, \psi, \omega) = -2 \int_\Omega (\widetilde{u} - u)\psi \, \mathrm{d}x \ , \quad \forall \psi$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

dual problem ∂_u:

$$J_u(\alpha, u)(\psi) - a_u(\alpha, u, \omega)(\psi) = 0 \ , \quad \forall \psi$$

$$a(\alpha, \psi, \omega) = -2 \int_\Omega (\widetilde{u} - u)\psi \, \mathrm{d}x \ , \quad \forall \psi$$

$$\int_\Omega \psi_t \omega + \alpha \nabla \psi \cdot \nabla \omega \, \mathrm{d}x = -2 \int_\Omega (\widetilde{u} - u)\psi \, \mathrm{d}x \ , \quad \forall \psi$$

$$-\omega_t = \nabla \cdot (\alpha \nabla \omega) - 2(\widetilde{u} - u) \ , \quad t : T \to 0$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

control problem ∂_α:

$$J_\alpha(\alpha, u)(\chi) - a_\alpha(\alpha, u, \omega)(\chi) = 0 \quad , \quad \forall \chi$$

outlook – automated, adaptive calibration

$$L(\alpha, u, \omega) = J(\alpha, u) - a(\alpha, u, \omega) + l(\omega)$$

optimality system, $L'(\alpha, u, \omega) = 0$:

control problem ∂_α:

$$J_\alpha(\alpha, u)(\chi) - a_\alpha(\alpha, u, \omega)(\chi) = 0 \;, \quad \forall \chi$$

$$2\eta \int_\Omega \alpha \; \chi \; \mathrm{d}x = \int_\Omega \nabla u \cdot \nabla \omega \; \chi \; \mathrm{d}x \;, \quad \forall \chi$$

$$\chi = 1 : \quad 2\eta \int_\Omega \alpha \; \mathrm{d}x = \int_\Omega \nabla u \cdot \nabla \omega \; \mathrm{d}x$$

conclusion: there is a free lunch!

solve

1. primal
2. dual (linear problem)
3. control

- *self calibrating, adaptive models*
- *adaptivity for free!*