Numerical Methods for Interfaces in Viscous Fluid Flow and Regularizing Effects in Parabolic Difference Equations

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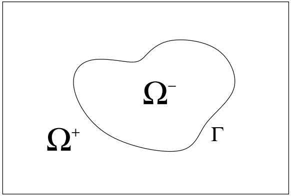
(1) (with Anita Layton) A second-order accurate method for a moving elastic interface with zero thickness in viscous fluid, original problem for Peskin's immersed boundary method

(2) Estimates in maximum norm for
finite difference versions of $u_t = \Delta u + f$
u and spatial differences bounded in L^∞ by $\|f\|_{L^\infty}$

Estimates in (2) relate to accuracy in (1)

Prototype Problem, Interface in Viscous Fluid

Navier-Stokes equations
interface Γ : $\mathbf{X}(\alpha, t)$
$\alpha =$ material coordinate
$s =$ arclength at current time
restoring force on Γ acts on fluid
periodic b.c.'s on box



$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f} \delta_\Gamma \, ,$$

$$\nabla \cdot \mathbf{u} = 0 \, , \qquad \boldsymbol{\tau} = \text{ unit tangent,}$$

$$\mathbf{f}(s,t) = \frac{\partial}{\partial s} \left(T(s,t) \boldsymbol{\tau}(s,t) \right) \, ,$$

$$T(s,t) = T_0 \left(\left| \frac{\partial \mathbf{X}}{\partial \alpha} \right| - 1 \right)^+ \, .$$

interfacial force amounts to jumps in $\nabla \mathbf{u}$ and p:

Jump conditions at the interface Γ:

$$[p] = \mathbf{f} \cdot \mathbf{n}, \quad \left[\frac{\partial p}{\partial \mathbf{n}}\right] = \frac{\partial}{\partial s}\left(\mathbf{f} \cdot \boldsymbol{\tau}\right),$$

$$[\mathbf{u}] = 0, \quad \mu\left[\frac{\partial \mathbf{u}}{\partial \mathbf{n}}\right] = -\left(\mathbf{f} \cdot \boldsymbol{\tau}\right)\boldsymbol{\tau}.$$

Peskin's Immersed Boundary Method:
designed for this problem and generalizations
robust, many applications in biology
force on boundary replaced by smooth delta functions
force is spread to grid points
many improvements for accuracy and stability...
first order for sharp interface (zero thickness)
second order for layer (positive thickness)
C. Peskin, B. Griffith, Y. Mori

The jump conditions suggest use of the

immersed interface method of R. LeVeque and Z. Li

or the related method of A. Mayo

or boundary integrals, layer potentials

These methods work well for Stokes flow:

$$-\mu\Delta\mathbf{u} + \nabla p = \mathbf{f}\delta_\Gamma\,, \quad \nabla\cdot\mathbf{u} = 0$$

The jump conditions are **the same** as for Navier-Stokes:

$$[p] = \mathbf{f}\cdot\mathbf{n}, \quad \left[\frac{\partial p}{\partial \mathbf{n}}\right] = \frac{\partial}{\partial s}\left(\mathbf{f}\cdot\boldsymbol{\tau}\right),$$
$$[\mathbf{u}] = 0, \quad \mu\left[\frac{\partial \mathbf{u}}{\partial \mathbf{n}}\right] = -\left(\mathbf{f}\cdot\boldsymbol{\tau}\right)\boldsymbol{\tau}.$$

Velocity Decomposition (with A. Layton)

Navier-Stokes equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f} \delta_\Gamma \,, \quad \nabla \cdot \mathbf{u} = 0$$

Stokes equations:

$$0 = -\nabla p_s + \mu \Delta \mathbf{u}_s + \mathbf{f} \delta_\Gamma \,, \quad \nabla \cdot \mathbf{u}_s = 0$$

Set $\mathbf{u} = \mathbf{u}_s + \mathbf{u}_r$, $\mathbf{u}_s =$ "Stokes" part, $\mathbf{u}_r =$ "regular" part
Jump conditions are the same for $\mathbf{u}$ and $\mathbf{u}_s$
velocity continuous $\rightarrow$ material deriv continuous
The "regular" part $\mathbf{u}_r$ has zero jumps (to order considered)

Decomposition Equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f} \delta_\Gamma \,, \quad \nabla \cdot \mathbf{u} = \mathbf{0}$$

$$0 = -\nabla p_s + \mu \Delta \mathbf{u}_s + \mathbf{f} \delta_\Gamma \,, \quad \nabla \cdot \mathbf{u_s} = \mathbf{0}$$

Substitute $\mathbf{u} = \mathbf{u}_s + \mathbf{u}_r$, $p = p_s + p_r$,

$$\frac{\partial \mathbf{u}_r}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u}_r = -\nabla p_r + \mu \Delta \mathbf{u}_r + \mathbf{F}_b \,, \quad \nabla \cdot \mathbf{u}_r = 0 \,,$$

$$\mathbf{F}_b = -\frac{\partial \mathbf{u}_s}{\partial t} - \mathbf{u} \cdot \nabla \mathbf{u}_s$$

To solve for $\mathbf{u}$ at each time,

(1) Solve the Stokes equations for $\mathbf{u}_s$ using the immersed interface method or boundary integrals;

(2) Solve for the regular velocity $\mathbf{u}_r$ using the semi-Lagrangian method with the second-order BDF

Immersed Interface Method, R. LeVeque, Z. Li; A. Mayo

Poisson problem with interface:

$$\Delta u_- = F_- \quad \text{in } \Omega_-, \qquad \Delta u_+ = F_+ \quad \text{in } \Omega_+,$$
$$[u] = g_0 \quad \text{on } \Gamma, \qquad [\partial_n u] = g_1 \quad \text{on } \Gamma$$

Solve

$$\Delta^h u^h = F^h + C^h$$

$C^h = 0$ at regular grid points; truncation error $O(h^2)$

truncation error $= \Delta^h u^{exact} - F^{exact}$

$C^h \neq 0$ at irregular points, stencil crosses Γ

C^h found from jumps u, Du, $D^2 u$

determined by g_0, g_1,$F_\pm$; truncation error $O(h)$, not $O(h^2)$

Error $u^h - u = O(h^2)$ uniformly! $\nabla_h u$ almost as good!

Z. Li & K. Ito, The IIM..., SIAM, 2006

JTB and A. Layton, CAMCoS ('06), analysis and applications

Immersed Interface Method applied to Elastic Interface

R. LeVeque & Z. Li ('97) Stokes flow; three Poisson problems

$$-\mu\Delta\mathbf{u} + \nabla p = \mathbf{f}\delta_\Gamma \,, \quad \nabla\cdot\mathbf{u} = 0$$

Navier-Stokes with elastic interface:
Z. Li & M.-C. Lai ('01)
L. Lee & R. LeVeque ('03)
S. Xu & Z. J. Wang ('06)
D. Le, B. Khoo & J. Peraire ('06)
Z. Tan, D. Le, Z. Li, K. Lim, B. Khoo ('08)
For NSE, the IIM can be second-order accurate in space & time
but many correction terms for jumps are needed

Regular Velocity

$$\frac{D\mathbf{u}_r}{Dt} + \nabla p_r - \mu\Delta\mathbf{u}_r = \mathbf{F}_b \equiv -\frac{D\mathbf{u}_s}{Dt},$$

$$\nabla\cdot\mathbf{u} = 0, \qquad \frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla$$

$\mathbf{u}$ continuous at $\Gamma \implies D\mathbf{u}/Dt$ continuous at Γ; same $\mathbf{u}_s$

$\mathbf{u}_r$, $D\mathbf{u}_r$, $D^2\mathbf{u}_r$ are continuous at Γ

e.g., Z. Li & M.-C. Lai ('01)

however, $\nabla\mathbf{u}$, $\nabla\mathbf{u}_s$, $\partial\mathbf{u}_s/\partial t$ have jumps

To solve for $\mathbf{u}_r$ on a grid,

we don't want to do something special at Γ;

it's better not to discretize the transport term;

we'd like to use a large time step;

we'd like to smooth high modes

(related to accuracy in the immersed interface method)

Semi-Lagrangian (CIR) Method

find values at new time t_{n+1} at grid points
material derivatives from backward characteristics

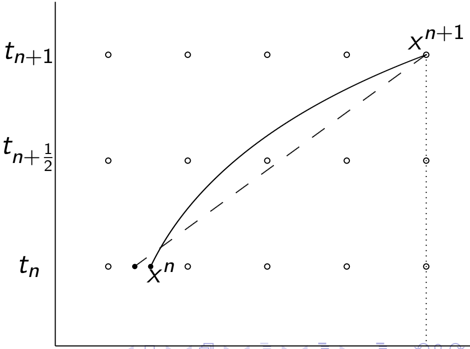
$$dx/dt = \mathbf{u}(x,t)\,, \quad x(t_{n+1}) = x^{n+1}$$

interpolate old value at "departure point" $x^n = x(t_n)$
error like $\Delta t^m + \Delta x^p / \Delta t$
Xiu & Karniadakis ('01); Biros, Ying & Zorin

$$\frac{D\mathbf{u}_r}{Dt} + \nabla p_r - \mu \Delta \mathbf{u}_r + \mathbf{F}_b\,,$$

$$\nabla \cdot \mathbf{u}_r = 0\,,$$

$$\mathbf{F}_b = -\frac{D\mathbf{u}_s}{Dt}$$



Computing the Regular Velocity

$$\frac{D\mathbf{u}_r}{Dt} + \nabla p_r - \mu\Delta\mathbf{u}_r = -\frac{D\mathbf{u}_s}{Dt}, \quad \nabla\cdot\mathbf{u}_r = 0$$

Second-order backward difference formula:

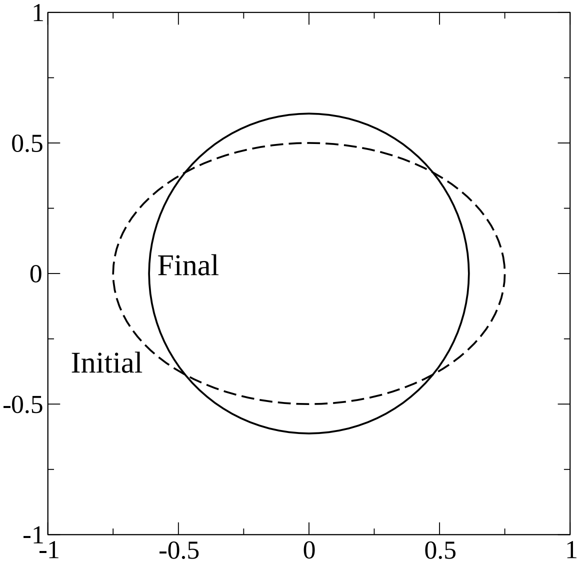
$$\frac{3\mathbf{u}_r^* - 4\tilde{\mathbf{u}}_r^n + \tilde{\mathbf{u}}_r^{n-1}}{2\Delta t} + \nabla p_r^n - \mu\Delta\mathbf{u}_r^* = \frac{3\mathbf{u}_s^{n+1} - 4\tilde{\mathbf{u}}_s^n + \tilde{\mathbf{u}}_s^{n-1}}{2\Delta t}$$

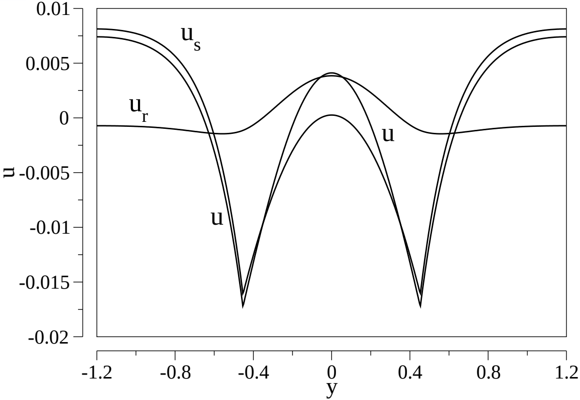
$$\mathbf{u}_r^{n+1} = \mathbb{P}\mathbf{u}_r^*,$$

$\mathbb{P}$ = approximate projection on div-free vectors
uses centered difference operators
amounts to pressure Poisson equation

Is this good enough for second-order accuracy?
$O(h^2)$ accuracy expected from immersed interface method
despite $O(h)$ truncation error at interface
Analysis partially justifies this...

Example 1. Relaxing or Oscillating Ellipse





$u =$ the x-component of fluid velocity at $x = 0.3$ and $t = 1.2$

$u = u_s + u_r =$ Stokes part plus regular part; $\mu = .1$

u and u_s have discontinuous normal derivative,

whereas u_r does not

Example 1. Convergence Test

initial semiaxes .7 and .5 , unstretched radius .5 , $T_0 = .2$

Errors in Area and Velocity, Grid Points and Interface

N	Area	L^2(grid)	L^∞(grid)	$L^2(\Gamma)$	$L^\infty(\Gamma)$
			$\mu = 0.1$		
80	5.291E-4	8.319E-4	1.036E-3	1.032E-3	1.176E-3
160	1.773E-4	3.026E-4	3.599E-4	2.366E-4	4.180E-4
320	5.299E-5	8.007E-5	1.160E-4	6.969E-5	1.237E-4
640	1.286E-5	1.300E-5	2.561E-5	1.462E-5	2.425E-5
			$\mu = 0.01$		
80	2.057E-3	3.734E-3	6.850E-3	1.995E-3	4.903E-3
160	6.903E-4	1.311E-3	2.822E-3	6.395E-4	1.560E-3
320	1.662E-4	3.156E-4	6.600E-4	1.674E-4	4.123E-4
640	4.053E-5	8.659E-5	1.548E-4	6.081E-5	1.025E-4

Error in area is compared to the exact value.

Errors in velocity are compared to $N = 1280$.

Stiff Boundary Force

Large tension coeff't T_0 requires small time step if explicit
Fractional time stepping is natural here
with small time steps for Stokes part

Decomposition $u = u_s + u_r$ puts interfacial force in Stokes part
To move Γ with Stokes, velocity is needed only on Γ
Stokes velocity on Γ in 2D free space
is easily written as a boundary integral

$$\mathbf{u}_s{}^{free} = \int_\Gamma V(\mathbf{X} - \mathbf{y})\mathbf{f}(\mathbf{y})ds(\mathbf{y}).$$

$$V_{ij}(\mathbf{x}) = -\frac{\delta_{ij}}{4\pi}\log|\mathbf{x}| + \frac{\mathbf{x}_i\mathbf{x}_j}{4\pi|\mathbf{x}|^2}$$

Need corrections for periodic b.c. and regular part

Fractional Time Steps

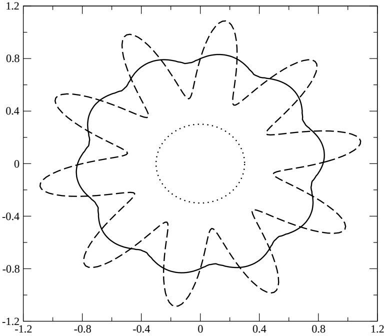
On small time steps

- Compute free-space Stokes velocity on Γ
- Correct for b.c. (extrapolate in time, interpolate in space)
- Add regular velocity (extrap. in time, interp. in space)
- Advance Γ using corrected velocity
- Update interfacial force

On large time step

- Solve Stokes eq'ns for $\mathbf{u}_s, p_s$ with periodic b.c.'s using IIM
- Solve Stokes eq'ns in free space using IIM
- Subtract two Stokes sol'ns for use with small steps
- Find regular velocity $\mathbf{u}_r$ using semi-Lagrangian method
- Add to get velocity $\mathbf{u} = \mathbf{u}_s + \mathbf{u}_r$.

Example 2



Tension coefficient $T_0 = 10$
viscosity $\mu = .1$

Case 1: Time step $= h$.
Unstable.

Case 2: Time step $= h/10$.
Stable.

Case 3: Small step $= h/10$,
Big step $= h$.
Stable, with similar accuracy

To Do

For stiff boundary force or more general forces,
we need implicit boundary motion.
Use approx'n to important part of boundary update ?
"Removing the stiffness", Hou, Lowengrub, Shelley ('94)
Kropinski ('01); Hou & Shi ('08)

More general boundary motion, esp. for 3D
JTB & Strain ('08)
J. Wilson, Ph.D. student

Maximum Norm Estimates for Parabolic Difference Equations with Gain in Regularity

for $u_t = \Delta u$ in $\mathbb{R}^d \times [0, T]$
discretize on square grid, spacing h, time step k
use Δ_h, usual second-order Laplacian, $\Delta_h = \sum_{\nu=1}^d D_\nu^+ D_\nu^-$
use implicit time stepping, $k = O(h)$
for single step, $u^n = s(k\Delta_h)^n u^0$
Backward Euler:

$$u^{n+1} - u^n = k\Delta_h u^{n+1}\,, \qquad s(k\Delta_h) = (1 - k\Delta_h)^{-1}$$

Crank-Nicolson:

$$\begin{aligned} u^{n+1} - u^n &= (k/2)(\Delta_h u^{n+1} + \Delta_h u^n)\,, \\ s(k\Delta_h) &= (1 + k\Delta_h/2)(1 - k\Delta_h/2)^{-1} \end{aligned}$$

best results for a second-order L-stable method (not CN)
including BDF2, second-order backward difference formula

for a single-step method, $u^n = s(k\Delta_h)^n u^0$
assume the method is L-stable, i.e.

$|s(z)| \leq 1$ for Re $z \leq 0$ (A-stable)

$s(z) \to 0$ as $z \to \infty$

Examples: Twizell, Gume, Arigu (TGA, an improvement of CN); one SDIRK2 (Runge-Kutta); BDF2 (but multi-step)
(CN does not have $s(\infty) = 0$.)

Main Result. For L-stable case, with operator norm on $L^\infty(\mathbb{R}_h^d)$,

$$\|s^n(k\Delta_h)\| \leq C_0$$
$$\|D_h s^n(k\Delta_h)\| \leq C_1 (nk)^{-1/2}$$
$$\|D_h^2 s^n(k\Delta_h)\| \leq C_2 (nk)^{-1}(1 + |\log h| + |\log nk|)$$

for $nk \leq T$, with constants independent of h and k.

For CN, s^n is bounded, but not differences.

Related work: Aronson ('63), Widlund ('66) for $k = O(h^2)$;
Ashyralyev & Sobolevskii; Thomée et al. for finite elements

Error Estimates for Parabolic Equations

Apply Main Result to a nonhomogeneous equation:

$$u_t = \Delta u + f, \quad u(\cdot, 0) = 0$$

with a method as above. E.g. for CN,

$$u^{n+1} = s(k\Delta_h)u^n + k(1 - \Delta_h/2)^{-1} f^{n+1/2}$$

For an L-stable method, u, $D_h u$, $D_h^2 u$ are bounded in max norm:

$$\|u^n\| + \|D_h u^n\| \le C_1 \sup_{t \le T} \|f(\cdot, t)\|$$

$$\|D_h^2 u^n\| \le C_2 \left(1 + |\log h|^2\right) \sup_{t \le T} \|f(\cdot, t)\|$$

For CN, first is true, second is not.

Interpretation: $u^{\text{computed}} - u^{\text{exact}}$ and differences are bounded by maximum truncation error.

Application to interfaces

Lemma. Suppose a grid function f is supported near an interface. Then $f = F_0 + \sum_{\nu=1}^{d} D_\nu^- F_\nu$, with $\|F_\nu\| \leq Ch\|f\|$.

Suppose we solve $u_t = \Delta u$ in a periodic box
with (known) jumps at a (known) interface.
Suppose the truncation error is
$O(h)$ near interface, $O(h^2)$ away.
The error equation ($e = u^{\text{computed}} - u^{\text{exact}}$) looks like

$$e_t = \Delta e + DF + O(h^2), \qquad F = O(h^2)$$

Using the Main Result and Lemma, we get
For CN, $e = O(h^2)$ uniformly.
For L-stable methods, $e = O(h^2)$,
and $D_h e = O(h^2 |\log h|^2)$ uniformly.

applies to linear convection-diffusion; full problem is harder

Proof of the Main Result

$$\|s^n(k\Delta_h)\| \le C_0$$
$$\|D_h s^n(k\Delta_h)\| \le C_1(nk)^{-1/2}$$
$$\|D_h^2 s^n(k\Delta_h)\| \le C_2(nk)^{-1}(1 + |\log h| + |\log nk|)$$

Use the point of view of analytic semigroups, as in
Thomée, Galerkin FEM for Parabolic Problems
Ashyralyev & Sobolevskii, ...Parabolic Difference Eq'ns

Step 1. Estimate $D_h^m e^{\Delta_h t}$ on $L^\infty(\mathbb{R}_h^d)$
Use $g_t = \Delta_h g, \quad g(jh,0) = \delta_{j0}$
Estimate $D_h^m g$ in discrete L^1 in Fourier transform (F. John, '52)
Show $\|D_h^m e^{\Delta_h t}\| \le C_m |t|^{-m/2}$ for **complex** t,
t in a sector in the right half plane,
$\{t = t_1 + it_2 : t_1 > 0, |t_2| \le Mt_1\}$

Proof of the Main Result

Step 2. Estimate the resolvent of Δ_h:

$$(z - \Delta_h)^{-1} = \int_0^\infty e^{-zt} e^{\Delta_h t}\, dt$$

Moving the ray in the t-sector, we get

$$\begin{aligned} \|(z - \Delta_h)^{-1}\| &\leq C_0 |z|^{-1}, \\ \|D_h(z - \Delta_h)^{-1}\| &\leq C_1 |z|^{-1/2}, \\ \|D_h^2(z - \Delta_h)^{-1}\| &\leq C_2(1 + |\log|z|| + |\log h|) \end{aligned}$$

for z outside a sector about $z < 0$

For periodic functions, mean value zero,

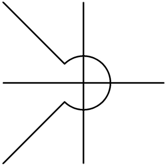
$$\|(\Delta_h)^{-1}\| \leq C_0\,,\ \|D_h(\Delta_h)^{-1}\| \leq C_1\,,\ \|D_h^2(\Delta_h)^{-1}\| \leq C_2(1 + |\log h|)$$

Proof of the Main Result

Step 3. Estimate $s(k\Delta_h)^n$ and differences:

$$D_h^\alpha s(k\Delta_h)^n = \frac{1}{2\pi i}\int_\Gamma s(z)^n D_h^\alpha (z - k\Delta_h)^{-1} dz$$

use contour Γ, radius $O(1/n)$
use resolvent estimates
from Step 2
use assumptions on s:



$s(z)$ analytic in a sector about $z < 0$,
$s(z) = 1 + z + O(z^2)$ as $z \to 0$,
$|s(z)| \le (1 + c_1|z|)^{-1}$, z in sector about $z < 0$
(from consistency and L-stability)

More General Parabolic Operators?

Michael Pruitt, Ph.D. thesis
Step 1 has to be completely different,
Estimate $\exp(A_h t)$, A_h an elliptic operator
For variable coefficients, use a discrete parametrix...

References

preprints at www.math.duke.edu/faculty/beale

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