Operator splitting techniques

Divide-and-conquer strategy: decompose unwieldy (systems of) PDEs into simpler subproblems and treat them individually using specialized numerical algorithms

Differential splitting

$$\frac{\partial u}{\partial t} + \mathcal{L}u = 0, \quad \mathcal{L} = \sum_{s=1}^{S} \mathcal{L}_s$$

Discretization order: time, space (operator splitting is applied to $\mathcal{L}$ before the discretization in space)

$\mathcal{L}_s$ represent physical phenomena (convection, diffusion, reaction etc.) BC are needed for each subproblem

Objective: decoupling of physical effects in complex IBVPs

Algebraic splitting

$$\frac{\partial u}{\partial t} + Lu = 0, \qquad L = \sum_{s=1}^{S} L_s$$

Discretization order: space, time (operator splitting is applied to $L = \mathcal{L}_h$ resulting from the space discretization)

L_s represent discrete operators (sparse matrices of arbitrary origin) BC are built into L *beforehand*

Objective: segregated solution of the (semi-)discretized equations

First-order operator splitting

Initial value problem $\quad \frac{\partial u}{\partial t} + \mathcal{L}u = 0 \quad \text{in } (0,T) \qquad u(0) = u_0$

(Marchuk-)Yanenko method $\quad \mathcal{L} = \sum_{s=1}^{S} \mathcal{L}_s \quad$ (differential or algebraic)

$$\frac{\partial u^{(s)}}{\partial t} + \mathcal{L}_s u^{(s)} = 0 \qquad \text{in } (t^n, t^{n+1}) \qquad s = 1, \ldots, S$$

$$u^{(s)}(t^n) = u^{(s-1)}(t^{n+1}), \quad u^{(0)}(t^{n+1}) = u^n, \quad u^{n+1} = u^{(S)}(t^{n+1})$$

- subproblems can be discretized independently using different methods
- the splitting error is $\mathcal{O}(\Delta t)$ so that a first-order time-stepping will do
- it is possible to treat some subproblems explicitly and some implicitly
- substepping (different time steps for different subproblems) is feasible

Remark. The decomposition of $\mathcal{L}$ is non-unique: $\quad \mathcal{L} = \sum_{s=1}^{S} \mathcal{L}_s = \sum_{s=1}^{\tilde{S}} \tilde{\mathcal{L}}_s$

Yanenko splitting in the case $S = 2$

Initial value problem

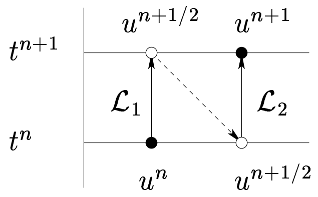
$$\frac{\partial u}{\partial t} + \mathcal{L}u = f, \qquad \mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$$

Fractional-step method

$$u^n \longrightarrow u^{n+1/2} \longrightarrow u^{n+1}$$

Subproblems discretized in time by the backward Euler method

1. $$\frac{u^{n+1/2} - u^n}{\Delta t} + \mathcal{L}_1 u^{n+1/2} = 0, \qquad u^{n+1/2} = [\mathcal{I} + \Delta t \mathcal{L}_1]^{-1} u^n$$
2. $$\frac{u^{n+1} - u^{n+1/2}}{\Delta t} + \mathcal{L}_2 u^{n+1} = f^n \qquad [\mathcal{I} + \Delta t \mathcal{L}_2] u^{n+1} = u^{n+1/2} + \Delta t f^n$$



Hence, $$[\mathcal{I} + \Delta t \mathcal{L}_1]([\mathcal{I} + \Delta t \mathcal{L}_2] u^{n+1} - \Delta t f^n) = u^n$$

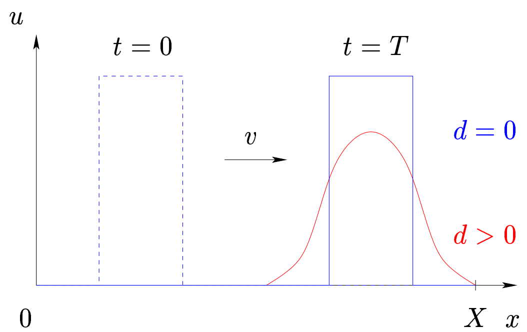
$$\frac{u^{n+1} - u^n}{\Delta t} + \mathcal{L} u^{n+1} = f^n + \Delta t \mathcal{L}_1 (f^n - \mathcal{L}_2 u^{n+1})$$

Remark. Yanenko splitting is first-order accurate and unconditionally stable if the discrete counterparts of $\mathcal{L}_1$ and $\mathcal{L}_2$ are nonnegative definite matrices

Example: 1D convection-diffusion equation

Convection-dominated problem

$$\begin{cases} \frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = d\frac{\partial^2 u}{\partial x^2} & \text{in } (0,X)\times(0,T) \\ u(0) = u(1) = 0, \quad u|_{t=0} = u_0 \end{cases}$$



Caution: standard Galerkin FEM is unstable!

Taylor series expansion $\quad u^{n+1} = u^n + \Delta t \left(\frac{\partial u}{\partial t}\right)^n + \frac{(\Delta t)^2}{2}\left(\frac{\partial^2 u}{\partial t^2}\right)^n + \mathcal{O}(\Delta t)^3$

Time derivatives $\quad \frac{\partial u}{\partial t} = -\mathcal{L}u, \quad \frac{\partial^2 u}{\partial t^2} = \mathcal{L}^2 u, \quad$ where $\mathcal{L} = v\frac{\partial}{\partial x} - d\frac{\partial^2}{\partial x^2}$

It is obvious that Lax-Wendroff/Taylor-Galerkin methods with a fourth-order operator $\mathcal{L}^2$ are not applicable to (multi-)linear finite element approximations

Crank-Nicolson scheme in incremental form

$$\frac{\partial^2 u}{\partial t^2} = -\mathcal{L}\frac{\partial u}{\partial t} = -\mathcal{L}\frac{u^{n+1}-u^n}{\Delta t} + \mathcal{O}(\Delta t) \quad \Rightarrow \quad \left[\mathcal{I} + \frac{\Delta t}{2}\mathcal{L}\right]\frac{u^{n+1}-u^n}{\Delta t} = -\mathcal{L}u^n$$

Remark. Stabilization term vanishes in the steady state limit $u^{n+1} = u^n$

Example: 1D convection-diffusion equation

Yanenko splitting for the convection-diffusion operator $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$

1. Convection step: Euler-TG method (explicit, third-order accurate)

$$\left[\mathcal{I} - \frac{(\Delta t)^2}{6}\mathcal{L}_1^2\right]\frac{u^{n+1/2} - u^n}{\Delta t} = -\mathcal{L}_1 u^n + \frac{\Delta t}{2}\mathcal{L}_1^2 u^n, \qquad \text{where} \quad \mathcal{L}_1 = v\frac{\partial}{\partial x}$$

   The pure convection equation is hyperbolic so that the boundary conditions should be imposed only at the inlet: $u(0) = 0$ if $v > 0$, $u(1) = 0$ if $v < 0$

2. Diffusion step: Crank-Nicolson scheme (implicit, second-order accurate)

$$\left[\mathcal{I} + \frac{\Delta t}{2}\mathcal{L}_2\right]\frac{u^{n+1} - u^{n+1/2}}{\Delta t} = -\mathcal{L}_2 u^{n+1/2}, \qquad \text{where} \quad \mathcal{L}_2 = -d\frac{\partial^2}{\partial x^2}$$

   The pure diffusion equation is parabolic so that the homogeneous boundary conditions are to be prescribed at both endpoints: $u(0) = u(1) = 0$

Remark. The overall temporal accuracy is $\mathcal{O}(\Delta t)$ due to the splitting error

Example: coordinate splitting in two dimensions

Consider the PDE $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + \beta \frac{\partial^2 u}{\partial y^2}$ discretized in space by CDS

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\Delta x)^2}, \qquad \left(\frac{\partial^2 u}{\partial y^2}\right)_{i,j} \approx \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{(\Delta y)^2}$$

Problem: the resulting matrix is banded but not tridiagonal (5-point stencil)

<u>Alternating Direction Implicit (ADI) method</u>

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$$

1. Sweep in the $x-$direction $\quad \mathcal{L}_1 = \alpha \frac{\partial^2}{\partial x^2}$

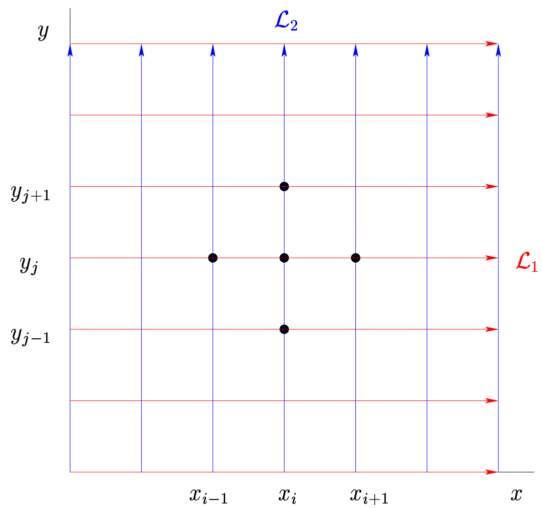
$$\frac{u_{i,j}^{n+1/2} - u_{i,j}^{n}}{\Delta t} = \alpha \frac{u_{i-1,j}^{n+1/2} - 2u_{i,j}^{n+1/2} + u_{i+1,j}^{n+1/2}}{(\Delta x)^2}$$

1D subproblems along the line $y_j = const$

2. Sweep in the $y-$direction $\quad \mathcal{L}_2 = \beta \frac{\partial^2}{\partial y^2}$

$$\frac{u_{i,j}^{n+1} - u_{i,j}^{n+1/2}}{\Delta t} = \beta \frac{u_{i,j-1}^{n+1} - 2u_{i,j}^{n+1} + u_{i,j+1}^{n+1}}{(\Delta y)^2}$$

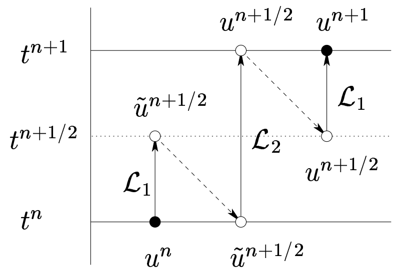
1D subproblems along the line $x_i = const$



Second-order operator splitting

Initial value problem $\qquad \mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$

$$\frac{\partial u}{\partial t} + \mathcal{L}u = 0 \quad \text{in } (0, T) \qquad u(0) = u_0$$



Symmetrized Strang splitting $\qquad S = 2$

1. $\frac{\partial u}{\partial t} + \mathcal{L}_1 u = 0 \quad \text{in } (t^n, t^{n+1/2}) \qquad u(t^n) = u^n \longrightarrow \tilde{u}^{n+1/2} = u(t^{n+1/2})$
2. $\frac{\partial u}{\partial t} + \mathcal{L}_2 u = 0 \quad \text{in } (t^n, t^{n+1}) \qquad u(t^n) = \tilde{u}^{n+1/2} \longrightarrow u^{n+1/2} = u(t^{n+1})$
3. $\frac{\partial u}{\partial t} + \mathcal{L}_1 u = 0 \quad \text{in } (t^{n+1/2}, t^{n+1}) \qquad u(t^{n+1/2}) = u^{n+1/2} \longrightarrow u^{n+1} = u(t^{n+1})$

- Strang splitting is second-order accurate and unconditionally stable if the discrete counterparts of $\mathcal{L}_1$ and $\mathcal{L}_2$ are positive definite matrices
- time-stepping of (at least) second order is mandatory for all subproblems
- for $S > 2$ the operators can be grouped in different ways, e.g. as follows

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 = (\mathcal{L}_1 + \mathcal{L}_2) + \mathcal{L}_3 = \mathcal{L}_1 + (\mathcal{L}_2 + \mathcal{L}_3) = \mathcal{A}_1 + \mathcal{A}_2$$

Second-order operator splitting

Initial value problem

$$\frac{\partial u}{\partial t} + \mathcal{L}u = f, \quad u(0) = u_0$$

Fractional step method $\quad S = 2$

$$u^n \longrightarrow u^{n+1/4} \longrightarrow u^{n+1/2} \longrightarrow u^{n+1}$$

<u>Predictor-corrector scheme</u> $\quad \mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 \quad$ (differential or algebraic)

1. $\frac{u^{n+1/4}-u^n}{\Delta t/2} + \mathcal{L}_1 u^{n+1/4} = f^{n+1/2}$
2. $\frac{u^{n+1/2}-u^{n+1/4}}{\Delta t/2} + \mathcal{L}_2 u^{n+1/2} = 0$
3. $\frac{u^{n+1}-u^n}{\Delta t} + \mathcal{L}u^{n+1/2} = f^{n+1/2}$

- first-order accurate Yanenko splitting is employed to predict u at $t^{n+1/2}$
- the explicit midpoint rule corrector yields a second-order accurate u^{n+1}

Elimination of $u^{n+1/4}$ gives $\quad \frac{u^{n+1/2}-u^n}{\Delta t} + \frac{1}{2}\mathcal{L}u^{n+1/2} + \frac{\Delta t}{4}\mathcal{L}_1\mathcal{L}_2 u^{n+1/2} = \frac{1}{2}f^{n+1/2}$

$$\mathcal{L}u^{n+1/2} = f^{n+1/2} - \frac{u^{n+1}-u^n}{\Delta t} \quad \Rightarrow \quad u^{n+1/2} = \frac{u^{n+1}+u^n}{2} - \frac{(\Delta t)^2}{4}\mathcal{L}_1\mathcal{L}_2 u^{n+1/2}$$

Hence, $\quad \frac{u^{n+1}-u^n}{\Delta t} + \mathcal{L}\left(\frac{u^{n+1}+u^n}{2}\right) = f^{n+1/2} + \frac{(\Delta t)^2}{4}\mathcal{L}\mathcal{L}_1\mathcal{L}_2 u^{n+1/2}, \quad$ where

$$u^{n+1/2} = \left(\mathcal{I} + \tfrac{\Delta t}{2}\mathcal{L}_2\right)^{-1}\left(\mathcal{I} + \tfrac{\Delta t}{2}\mathcal{L}_1\right)^{-1}\left(u^n + \tfrac{\Delta t}{2} f^{n+1/2}\right) = u^n + \mathcal{O}(\Delta t)$$

Second-order operator splitting

Predictor-corrector $\approx$ Crank-Nicolson up to the second order

$$\frac{u^{n+1}-u^n}{\Delta t} + \mathcal{L}\left(\frac{u^{n+1}+u^n}{2}\right) = f^{n+1/2} + \frac{(\Delta t)^2}{4}\mathcal{L}\mathcal{L}_1\mathcal{L}_2 u^n + \mathcal{O}(\Delta t)^3$$

unconditionally stable, at least if the discrete operators are positive-definite

Peaceman-Rachford scheme $\quad u^n \longrightarrow u^{n+1/2} \longrightarrow u^{n+1}$

1. $\frac{u^{n+1/2}-u^n}{\Delta t/2} + \mathcal{L}_1 u^{n+1/2} = f^{n+1/2} - \mathcal{L}_2 u^n$
2. $\frac{u^{n+1}-u^{n+1/2}}{\Delta t/2} + \mathcal{L}_2 u^{n+1} = f^{n+1/2} - \mathcal{L}_1 u^{n+1/2}$

popular ADI solver

second-order accurate, unconditionally stable for $\mathcal{L}_i = \frac{\partial^2}{\partial x_i^2}$ in 2D (not in 3D)

Douglas-Rachford scheme $\quad u^n \longrightarrow u^{n+1/2} \longrightarrow u^{n+1}$

1. $\frac{u^{n+1/2}-u^n}{\Delta t} + \mathcal{L}_1 u^{n+1/2} = f^n - \mathcal{L}_2 u^n$
2. $\frac{u^{n+1}-u^{n+1/2}}{\Delta t} + \mathcal{L}_2 u^{n+1} = \mathcal{L}_2 u^n$

can be generalized to the case $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3$

first-order accurate but unconditionally stable for $\mathcal{L}_i = \frac{\partial^2}{\partial x_i^2}$ in 2D and in 3D

Second-order operator splitting

Iliin's generalization   Let $\tau = \frac{\Delta t}{1+\rho}$,   where $\rho \in (-1, 1]$ is a parameter

1. $\frac{u^{n+1/2}-u^n}{\tau} + \mathcal{L}_1 u^{n+1/2} = f^{n+1/2} - \mathcal{L}_2 u^n$ DR scheme for $\rho = 0$
2. $\frac{u^{n+1}-u^{n+1/2}}{\tau} + \mathcal{L}_2(u^{n+1} - u^n) = \rho \frac{u^{n+1/2}-u^n}{\tau}$ PR scheme for $\rho = 1$

Rewrite (1) as $\frac{u^{n+1/2}-u^n}{\tau} + \mathcal{L}_1(u^{n+1/2} - u^n) = f^{n+1/2} - \mathcal{L}u^n$, $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$

Rewrite (2) as $\frac{u^{n+1}-u^n}{\tau} + \mathcal{L}_2(u^{n+1} - u^n) = (1+\rho)\frac{u^{n+1/2}-u^n}{\tau}$ and substitute

the ratio $\frac{u^{n+1/2}-u^n}{\tau} = (\mathcal{I} + \tau\mathcal{L}_1)^{-1}(f^{n+1/2} - \mathcal{L}u^n)$ into the right-hand side

This yields $(\mathcal{I} + \tau\mathcal{L}_1)(\mathcal{I} + \tau\mathcal{L}_2)(u^{n+1} - u^n) = \tau(1+\rho)(f^{n+1/2} - \mathcal{L}u^n)$

$$\tau = \frac{\Delta t}{1+\rho} \quad \Rightarrow \quad \frac{u^{n+1}-u^n}{\Delta t} + \mathcal{L}\left(\frac{u^{n+1}+\rho u^n}{1+\rho}\right) = f^{n+1/2} - \frac{(\Delta t)^2}{(1+\rho)^2}\mathcal{L}_1\mathcal{L}_2\left(\frac{u^{n+1}-u^n}{\Delta t}\right)$$

Properties: Iliin's method is second-order accurate for $\rho = 1$ (Peaceman-Rachford) and first-order accurate otherwise, unconditionally stable for any $\rho \in (-1, 1]$

Second-order operator splitting

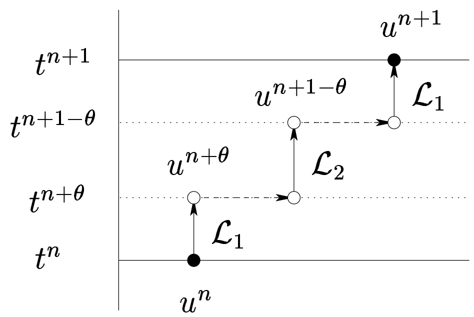
<u>Glowinski's fractional-step $\theta-$scheme</u>

Parameter $0 < \theta < \frac{1}{2}$

1. $\frac{u^{n+\theta}-u^n}{\theta\Delta t} + \mathcal{L}_1 u^{n+\theta} = f^n - \mathcal{L}_2 u^n$

2. $\frac{u^{n+1-\theta}-u^{n+\theta}}{(1-2\theta)\Delta t} + \mathcal{L}_2 u^{n+1-\theta} = f^{n+\theta} - \mathcal{L}_1 u^{n+\theta}$

3. $\frac{u^{n+1}-u^{n+1-\theta}}{\theta\Delta t} + \mathcal{L}_1 u^{n+1} = f^{n+1-\theta} - \mathcal{L}_2 u^{n+1-\theta}$



- second-order accurate for $\theta = 1 - \frac{\sqrt{2}}{2}$ and first-order accurate otherwise
- a complete analysis of stability is not available but the results are good
- strongly A-stable if used as a time-stepping method (without splitting)
- particularly useful for the treatment of the Navier-Stokes equations

Remark. The notions "operator splitting" and "fractional step methods" are used as synonyms in the literature. In fact, the former should refer to the decomposition $\mathcal{L} = \sum_s \mathcal{L}_s$ underlying a particular time-stepping scheme denoted by the latter

Incompressible flow problems

Navier-Stokes equations

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nu \Delta \mathbf{u}$$

$$\nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega \times (0, T)$$

Boundary condition

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{g} \quad \text{on } \Gamma \times (0, T)$$

Initial condition

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad \text{in } \Omega$$

Solvability conditions $\quad \nabla \cdot \mathbf{u}_0 = 0, \quad \mathbf{n} \cdot \mathbf{u}_0 = \mathbf{n} \cdot \mathbf{g}, \quad \int_\Gamma \mathbf{n} \cdot \mathbf{g} \, ds = 0$

- this is a coupled PDE system for the velocity $\mathbf{u}$ and pressure p
- the pressure is determined up to an arbitrary additive constant and acts as a *Lagrange multiplier* for the incompressibility constraint

Pressure Poisson equation (can be used instead of $\nabla \cdot \mathbf{u} = 0$)

$$-\Delta p = \nabla \cdot [\mathbf{u} \cdot \nabla \mathbf{u} - \nu \Delta u] \quad \text{in } \Omega, \qquad \mathbf{n} \cdot \nabla p = \mathbf{n} \cdot \left[\nu \Delta \mathbf{u} - \mathbf{u} \cdot \nabla \mathbf{u} - \frac{\partial \mathbf{u}}{\partial t}\right] \quad \text{on } \Gamma$$

Caution: the approximation spaces for $\mathbf{u}$ and p should satisfy the *LBB stability condition* or the discretized equations should be stabilized by extra terms

Chorin's projection scheme

Idea: decouple $\mathbf{u}$ and p and separate convection-diffusion from incompressibility

Fractional-step method $\qquad \mathbf{u}^n \longrightarrow \mathbf{u}^{n+1/2} \longrightarrow (\mathbf{u}^{n+1}, p^{n+1})$

1. Omit the pressure gradient in the momentum equation, disregard the incompressibility constraint and solve the viscous Burgers equation

$$\frac{\mathbf{u}^{n+1/2} - \mathbf{u}^n}{\Delta t} + \mathbf{u}^{n+1/2} \cdot \nabla \mathbf{u}^{n+1/2} = \nu \Delta \mathbf{u}^{n+1/2}, \qquad \mathbf{u}^{n+1/2} = \mathbf{g} \quad \text{on } \Gamma$$

2. Project the velocity $\mathbf{u}^{n+1/2}$ onto the subspace of solenoidal functions

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1/2}}{\Delta t} = -\nabla p^{n+1} \qquad \text{Inviscid flow} \Rightarrow \text{tangential slip}$$

$$\nabla \cdot \mathbf{u}^{n+1} = 0 \qquad \mathbf{n} \cdot \mathbf{u}^{n+1} = \mathbf{n} \cdot \mathbf{g} \quad \text{on } \Gamma$$

Poisson equation $\quad -\Delta p^{n+1} = -\frac{1}{\Delta t} \nabla \cdot \mathbf{u}^{n+1/2}, \quad \mathbf{n} \cdot \nabla p^{n+1} = 0 \quad \text{on } \Gamma$

- wrong BC results in a spurious pressure boundary layer of width $\mathcal{O}(\sqrt{\nu \Delta t})$
- Chorin's method is $\mathcal{O}(\Delta t)$, stable for equal-order interpolations if $\Delta t \geq Ch^2$

Example: three-step projection scheme

Fractional-step method $\quad \mathbf{u}^n \longrightarrow \mathbf{u}^{n+1/4} \longrightarrow \mathbf{u}^{n+1/2} \longrightarrow (\mathbf{u}^{n+1}, p^{n+1})$

1. Convection step: Lax-Wendroff (explicit, second-order accurate)

$$\frac{\mathbf{u}^{n+1/4}-\mathbf{u}^n}{\Delta t} = \partial_t \mathbf{u}^n + \frac{\Delta t}{2}\partial_{tt}\mathbf{u}^n, \qquad \mathbf{u}^{n+1/4} = \mathbf{g} \quad \text{at the inlet } \Gamma_{\text{in}}$$

Time derivatives $\quad \partial_t \mathbf{u} = -\mathbf{u}\cdot\nabla\mathbf{u}, \qquad$ where $\mathbf{u} = \mathbf{u}(\mathbf{x}, t) \quad \Rightarrow$

$$\partial_{tt}\mathbf{u} = -(\partial_t \mathbf{u})\cdot\nabla\mathbf{u} - \mathbf{u}\cdot\nabla(\partial_t\mathbf{u}) = (\mathbf{u}\cdot\nabla\mathbf{u})\cdot\nabla\mathbf{u} + \mathbf{u}\cdot\nabla(\mathbf{u}\cdot\nabla\mathbf{u})$$

Variational formulation $\quad \langle \mathbf{a}, \mathbf{b}\rangle := \int_\Omega \mathbf{a}\cdot\mathbf{b}\, d\mathbf{x}, \quad \langle \mathbf{a}, \mathbf{b}\rangle_\Gamma := \int_\Gamma \mathbf{a}\cdot\mathbf{b}\, ds$

$$\langle \mathbf{w}, \mathbf{u}^{n+1/4} - \mathbf{u}^n\rangle = -\Delta t \langle \mathbf{w}, \mathbf{u}^n\cdot\nabla\mathbf{u}^n\rangle - \frac{(\Delta t)^2}{2}\langle \mathbf{u}^n\cdot\nabla\mathbf{w}, \mathbf{u}^n\cdot\nabla\mathbf{u}^n\rangle$$
$$+\tfrac{(\Delta t)^2}{2}\left[\langle \mathbf{w}, (\mathbf{u}^n\cdot\nabla\mathbf{u}^n)\cdot\nabla\mathbf{u}^n\rangle - \langle \mathbf{w}\nabla\cdot\mathbf{u}^n, \mathbf{u}^n\cdot\nabla\mathbf{u}^n\rangle - \langle \mathbf{w}\mathbf{u}^n\cdot\mathbf{n}, \mathbf{u}^n\cdot\nabla\mathbf{u}^n\rangle_{\Gamma_{\text{out}}}\right]$$

Linear system $\quad M_C\mathbf{u}^{n+1/4} = \left[M_C + \Delta t K + \tfrac{(\Delta t)^2}{2} S\right]\mathbf{u}^n \quad$ can be solved by

a simple Jacobi-like iteration preconditioned by the lumped mass matrix M_L

Example: three-step projection scheme

2. Diffusion step: Crank-Nicolson scheme (implicit, second-order accurate)

$$\frac{\mathbf{u}^{n+1/2}-\mathbf{u}^{n+1/4}}{\Delta t}=\frac{\nu}{2}[\Delta\mathbf{u}^{n+1/2}+\Delta\mathbf{u}^{n+1/4}], \qquad \mathbf{u}^{n+1/2}=\mathbf{g} \quad \text{on } \Gamma$$

$$\langle\mathbf{w},\mathbf{u}^{n+1/2}-\mathbf{u}^{n+1/4}\rangle=-\tfrac{\Delta t}{2}\nu[\langle\nabla\mathbf{w},\nabla\mathbf{u}^{n+1/2}\rangle+\langle\nabla\mathbf{w},\nabla\mathbf{u}^{n+1/4}\rangle]$$

Linear system $\quad [M_C-\tfrac{\Delta t}{2}\nu L]\mathbf{u}^{n+1/2}=[M_C+\tfrac{\Delta t}{2}\nu L]\mathbf{u}^{n+1/4}$

3. Projection step: Pressure Poisson equation (elliptic, ill-conditioned)

$$-\Delta p^{n+1}=-\tfrac{1}{\Delta t}\nabla\cdot\mathbf{u}^{n+1/2} \qquad \langle\nabla q,\nabla p^{n+1}\rangle=-\tfrac{1}{\Delta t}\langle q,\nabla\cdot\mathbf{u}^{n+1/2}\rangle$$

$$\mathbf{n}\cdot\nabla p^{n+1}=0 \quad \text{on } \Gamma \qquad -Lp^{n+1}=-\tfrac{1}{\Delta t}\mathbf{B}^T\mathbf{u}^{n+1/2}$$

Remark. Advanced linear algebra tools (CG, multigrid) are needed.

Velocity update $\quad \mathbf{u}^{n+1}=\mathbf{u}^{n+1/2}-\Delta t\nabla p^{n+1} \qquad \mathbf{n}\cdot\mathbf{u}^{n+1}=\mathbf{n}\cdot\mathbf{g} \quad \text{on } \Gamma$

$$\langle\mathbf{w},\mathbf{u}^{n+1}-\mathbf{u}^{n+1/2}\rangle=-\Delta t\langle\mathbf{w},\nabla p^{n+1}\rangle \qquad \mathbf{u}^{n+1}=\mathbf{u}^{n+1/2}-\Delta t M_L^{-1}\mathbf{B}p^{n+1}$$

Van Kan's projection scheme

Fractional-step method $\qquad (\mathbf{u}^n, p^n) \longrightarrow \mathbf{u}^{n+1/2} \longrightarrow (\mathbf{u}^{n+1}, p^{n+1})$

1. Insert the old pressure gradient into the momentum equation, disregard the incompressibility constraint and solve the viscous Burgers equation

$$\frac{\mathbf{u}^{n+1/2}-\mathbf{u}^n}{\Delta t}+\frac{1}{2}[\mathbf{u}^{n+1/2}\cdot\nabla\mathbf{u}^{n+1/2}+\mathbf{u}^n\cdot\nabla\mathbf{u}^n]=-\nabla p^n+\frac{\nu}{2}[\Delta\mathbf{u}^{n+1/2}+\Delta\mathbf{u}^n]$$

subject to the no-slip boundary condition $\quad \mathbf{u}^{n+1/2}=\mathbf{g} \quad \text{on } \Gamma$

2. Project the velocity $\mathbf{u}^{n+1/2}$ onto the subspace of solenoidal functions

$$\frac{\mathbf{u}^{n+1}-\mathbf{u}^{n+1/2}}{\Delta t}=-\nabla q^{n+1} \qquad\qquad \boxed{p^{n+1}=p^n+2q^{n+1}}$$

$$\nabla\cdot\mathbf{u}^{n+1}=0 \qquad\qquad \mathbf{n}\cdot\mathbf{u}^{n+1}=\mathbf{n}\cdot\mathbf{g} \quad \text{on } \Gamma$$

Poisson equation $\quad -\Delta q^{n+1}=-\frac{1}{\Delta t}\nabla\cdot\mathbf{u}^{n+1/2}, \quad \mathbf{n}\cdot\nabla q^{n+1}=0 \quad \text{on } \Gamma$

- wrong BC results in a spurious pressure boundary layer of width $\mathcal{O}(\sqrt{\nu\Delta t})$
- Van Kan's method is $\mathcal{O}(\Delta t)^2$, stable for equal-order interpolations if $\Delta t \geq Ch$

Glowinski's splitting scheme

Fractional-step method with parameters $0 < \theta < \frac{1}{2}$ and $0 < \eta < 1$

1. Linear Stokes problem $\quad \mathbf{u}^n \longrightarrow (\mathbf{u}^{n+\theta}, p^{n+\theta}), \quad \mathbf{u}^{n+\theta} = \mathbf{g} \quad \text{on } \Gamma$

$$\frac{\mathbf{u}^{n+\theta} - \mathbf{u}^n}{\theta \Delta t} - \eta\nu\Delta\mathbf{u}^{n+\theta} + \nabla p^{n+\theta} = (1-\eta)\nu\Delta\mathbf{u}^n - \mathbf{u}^n \cdot \nabla\mathbf{u}^n$$

$\nabla \cdot \mathbf{u}^{n+\theta} = 0$ *can be solved by a variational CG algorithm*

2. Viscous Burgers equation $\quad \mathbf{u}^{n+\theta} \longrightarrow \mathbf{u}^{n+1-\theta}, \quad \mathbf{u}^{n+1-\theta} = \mathbf{g} \quad \text{on } \Gamma$

$$\frac{\mathbf{u}^{n+1-\theta} - \mathbf{u}^{n+\theta}}{(1-2\theta)\Delta t} - (1-\eta)\nu\Delta\mathbf{u}^{n+1-\theta} + \mathbf{u}^{n+1-\theta} \cdot \nabla\mathbf{u}^{n+1-\theta} = \eta\nu\Delta\mathbf{u}^{n+\theta} - \nabla p^{n+\theta}$$

convection and diffusion can be separated by means of operator splitting

3. Linear Stokes problem $\quad \mathbf{u}^{n+1-\theta} \longrightarrow (\mathbf{u}^{n+1}, p^{n+1}), \quad \mathbf{u}^{n+1} = \mathbf{g} \quad \text{on } \Gamma$

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^{n+1-\theta}}{\theta \Delta t} - \eta\nu\Delta\mathbf{u}^{n+1} + \nabla p^{n+1} = (1-\eta)\nu\Delta\mathbf{u}^{n+1-\theta} - \mathbf{u}^{n+1-\theta} \cdot \nabla\mathbf{u}^{n+1-\theta}$$

$\nabla \cdot \mathbf{u}^{n+1} = 0$ *can be solved by a variational CG algorithm*

Pressure Schur Complement methods

Discretized Navier-Stokes equations

$$A\mathbf{u} + \Delta t \mathbf{B} p = \mathbf{f}, \quad A = M_C - \theta \Delta t [K(\mathbf{u}) + \nu L]$$

$$\mathbf{u} = A^{-1}[\mathbf{f} - \Delta t \mathbf{B} p], \qquad \mathbf{B}^T \mathbf{u} = 0$$

$$\begin{bmatrix} A & \Delta t \mathbf{B} \\ \mathbf{B}^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix}$$

Substitution yields $\mathbf{B}^T A^{-1}[\mathbf{f} - \Delta t \mathbf{B} p] = 0 \quad \Rightarrow \quad -\mathbf{B}^T A^{-1} \mathbf{B} p = -\frac{1}{\Delta t} \mathbf{B}^T A^{-1} \mathbf{f}$

Richardson iteration for the PSC equation $\quad p^{(0)} = 0 \quad$ or $\quad p^{(0)} = p^n$

$$p^{(l+1)} = p^{(l)} + \alpha\, C^{-1}\, \mathbf{B}^T A^{-1} [\mathbf{f} - \Delta t \mathbf{B} p^{(l)}] \Delta t^{-1}, \qquad l = 0, \ldots, L$$

Additive preconditioners $\quad C^{-1} = \sum_i C_i^{-1} \approx [\mathbf{B}^T A^{-1} \mathbf{B}]^{-1} \quad$ (*Turek, 1995*)

Global MPSC $\quad C^{-1} := \alpha_M A_M^{-1} + \alpha_K A_K^{-1} + \alpha_L A_L^{-1} \quad$ operator splitting

$$A_M \approx \mathbf{B}^T M_C^{-1} \mathbf{B}, \quad A_K \approx \mathbf{B}^T K^{-1} \mathbf{B}, \quad A_L \approx \mathbf{B}^T L^{-1} \mathbf{B}$$

Local MPSC $\quad C^{-1} := \sum_i [\mathbf{B}^T_{|\Omega_i} A^{-1}_{|\Omega_i} \mathbf{B}_{|\Omega_i}]^{-1} \quad$ exact solution on patches Ω_i

Discrete projection methods

Observation: at high Reynolds numbers the time step must be small for accuracy reasons so that $A \approx M_C \approx M_L$ and $C := \mathbf{B}^T M_L^{-1} \mathbf{B}$ is a good preconditioner

Practical implementation of a global PSC cycle $\qquad l = 0, \dots, L$

1. Insert the last pressure iterate $p^{(l)}$ into the viscous Burgers equation

$$A\tilde{\mathbf{u}} = \mathbf{f} - \Delta t \mathbf{B} p^{(l)} \qquad \text{(linearized or nonlinear)}$$

   and compute an intermediate velocity $\tilde{\mathbf{u}}$ such that $\mathbf{B}^T \tilde{\mathbf{u}} \neq 0$ in general

2. Solve the discrete counterpart of the Pressure Poisson equation

$$-\mathbf{B}^T M_L^{-1} \mathbf{B} q = -\frac{1}{\Delta t} \mathbf{B}^T \tilde{\mathbf{u}} \qquad (p \text{ and } q \text{ may be piecewise constant})$$

3. Apply the pressure correction and render $\tilde{\mathbf{u}}$ discretely divergence-free

$$p^{(l+1)} = p^{(l)} + \alpha q, \qquad \mathbf{u}^{(l+1)} = \tilde{\mathbf{u}} - \Delta t M_L^{-1} \mathbf{B} q$$

Remark. For $L = 0$ this algorithm is equivalent to classical projection schemes (Chorin if $p^{(0)} = 0$, Van Kan if $p^{(0)} = p^n$) based on **discrete** operator splitting

Strongly coupled solution strategy

Basic iteration for a local MPSC method (*Turek, 1999*)

$$\begin{bmatrix} \mathbf{u}^{(l+1)} \\ p^{(l+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{u}^{(l)} \\ p^{(l)} \end{bmatrix} - \omega^{(l+1)} \sum_{i=1}^{N_p} \begin{bmatrix} \tilde{A}_{|\Omega_i} & \Delta t B_{|\Omega_i} \\ B^T_{|\Omega_i} & 0 \end{bmatrix}^{-1} \begin{bmatrix} \delta \mathbf{u}_i^{(l)} \\ \delta p_i^{(l)} \end{bmatrix},$$

where N_p denotes the total number of patches, $\omega^{(l+1)}$ is a relaxation parameter, and the global defect vector restricted to a single patch Ω_i is given by

$$\begin{bmatrix} \delta \mathbf{u}_i^{(l)} \\ \delta p_i^{(l)} \end{bmatrix} = \left(\begin{bmatrix} A & \Delta t B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u}^{(l)} \\ p^{(l)} \end{bmatrix} - \begin{bmatrix} \mathbf{g} \\ 0 \end{bmatrix} \right)_{|\Omega_i}$$

In practice, an auxiliary problem is solved for the solution increment

$$\begin{bmatrix} \tilde{A}_{|\Omega_i} & \Delta t B_{|\Omega_i} \\ B^T_{|\Omega_i} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}_i^{(l+1)} \\ q_i^{(l+1)} \end{bmatrix} = \begin{bmatrix} \delta \mathbf{u}_i^{(l)} \\ \delta p_i^{(l)} \end{bmatrix}, \qquad \begin{bmatrix} \mathbf{u}_{|\Omega_i}^{(l+1)} \\ p_{|\Omega_i}^{(l+1)} \end{bmatrix} = \begin{bmatrix} \mathbf{u}_{|\Omega_i}^{(l)} \\ p_{|\Omega_i}^{(l)} \end{bmatrix} - \omega^{(l+1)} \begin{bmatrix} \mathbf{v}_i^{(l+1)} \\ q_i^{(l+1)} \end{bmatrix}$$

Iterative treatment of nonlinearities

Nonlinear algebraic system $\boxed{A(u)u = f}$ must be solved iteratively

Defect correction scheme: compute successive approximations

$$u^{(m+1)} = u^{(m)} + \omega^{(m)}[\tilde{A}(u^{(m)})]^{-1}[f - A(u^{(m)})u^{(m)}], \qquad m = 0, 1, 2, \ldots$$

where $\tilde{A}(u^{(m)})$ is a suitable 'preconditioner' and $\omega^{(m)}$ is a relaxation parameter

Example. $\tilde{A}(u^{(m)}) := A(u^{(m)}), \quad \omega^{(m)} := 1 \quad \Rightarrow \quad A(u^{(m)})u^{(m+1)} = f$

Practical implementation of a defect correction step

1. Evaluate the residual $r^{(m)} = f - A(u^{(m)})u^{(m)}$ of the nonlinear system
2. Solve the auxiliary linear problem $\tilde{A}(u^{(m)})\delta u^{(m)} = r^{(m)}$ using a direct or iterative method (a moderate number of *inner iterations* will suffice)
3. Multiply the resulting solution increment $\delta u^{(m)}$ by the (under-)relaxation factor $\omega^{(m)}$ and apply it to the last iterate $u^{(m+1)} = u^{(m)} + \omega^{(m)}\delta u^{(m)}$