Concepts and Algorithms of Scientific and Visual Computing

–Partial Differential Equations–

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Partial Differential Equation

In contrast to an ordinary differential equation, a partial differential equation contains partial derivatives.

The corresponding Cauchy problem is analogously defined to the ordinary case.

The question of existence and uniqueness of the solution of an ordinary differential equation is answered by the Picard-Lindelöf theorem. It turned out, that this is much harder for partial differential equations, even in linear cases.

According to the Malgrange-Ehrenpreis theorem, linear partial differential equations with constant coefficients always have a solution. This can not be extended to linear partial differential equations with polynomial coefficients. In particular [Lewy 1957] presented an example of a linear partial differential equation with no solutions at all. In non-linear cases, the theory of partial differential equations shows significant gaps.

Partial Differential Equation

Partial differential equations are usually classified in three different categories.

Elliptic partial differential equations typically occur in the context of steady problems. Often, elliptic differential equations describe a state of extremal energy resulting from a variational principle.

Parabolic differential equations describe similar problems as elliptic ones, but in the in nonsteady case. Canonical examples are heat or diffusion equations.

Hyperbolic differential equations address oscillation processes. A typical equation of this kind is the wave equation.

Finite Difference Method (FDM)

Given a partial differential equation with two unknown multivariable functions, a finite difference approximation can be constructed using a grid with basis points

$$x_\mu = x_0 + \mu \Delta x, \quad y_\nu = y_0 + \nu \Delta y$$

for $\mu, \nu \in \{1, \dots, N\}$.

The partial derivatives are then replaced by finite expressions, e.g.

$$\begin{aligned}
\partial_x u(x_\mu, y_\nu) &\mapsto \frac{1}{\Delta x}(u_{\mu+1,\nu} - u_{\mu,\nu}), && \mathcal{O}(\Delta x) \\
\partial_x u(x_\mu, y_\nu) &\mapsto \frac{1}{2\Delta x}(u_{\mu+1,\nu} - u_{\mu-1,\nu}), && \mathcal{O}(\Delta x^2) \\
\partial_x \partial_y u(x_\mu, y_\nu) &\mapsto \frac{1}{4\Delta x \Delta y}(u_{\mu+1,\nu+1} - u_{\mu+1,\nu-1} - u_{\mu-1,\nu+1} - u_{\mu-1,\nu-1}), && \mathcal{O}(\Delta x \Delta y) \\
\partial_x^2 u(x_\mu, y_\nu) &\mapsto \frac{1}{\Delta x^2}(u_{\mu+1,\nu} - 2u_{\mu,\nu} + u_{\mu-1,\nu}), && \mathcal{O}(\Delta x^2)
\end{aligned}$$

$\partial_y u(x_\mu, y_\nu)$ and $\partial_y^2 u(x_\mu, y_\nu)$ analogously, in which $u_{\mu,\nu}$ approximates $u(x_\mu, y_\nu)$.

Navier-Stokes Equation

The state of a fluid can be described by the dynamic mapping

$$\mathbf{u} : (\mathbf{x}, t) \mapsto (u_1(\mathbf{x}, t), u_2(\mathbf{x}, t), u_3(\mathbf{x}, t))^\mathsf{T},$$

which for given time t and position $\mathbf{x} = (x_1, x_2, x_3)^\mathsf{T}$ returns the corresponding velocity field. It can be computed by solving the underlying Navier-Stokes equation

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla p = \mathbf{f} + \nu \nabla \cdot \nabla \mathbf{u}, \qquad (1)$$ [1]

in which the density of denoted by ρ, the pressure by p, the external net force with $\mathbf{f}$, and the kinematic viscosity by ν. To enforce incompressibility of the fluid, the additional constraint

$$\nabla \cdot \mathbf{u} = 0, \qquad (2)$$

which expresses that the vector field $\mathbf{u}$ is divergence free, is taken into account.[2]

[1] The vector Laplacian is similarly defined to its scalar counterpart and simply acts component-wise.

[2] We only consider incompressible fluids here, which do not change their density along trajectories.

Navier-Stokes Equation

We will briefly illustrate the derivation of Eq. (1) using an analogy to a particle system. For that assume, that the fluid is described using a set of particles. Its dynamical behavior can then be described using Newton's equations of motion, i.e.

$$m\mathcal{D}_t\mathbf{u} = \mathbf{F}$$

with a so-called material-derivation operator $\mathcal{D}$ and net force $\mathbf{F}$. To determine $\mathbf{F}$, we state, that an imbalance of higher pressure in a specific direction has to be taken into account. This can be measured by the gradient $-\nabla p$, so that its integral over the fluid volume V is given approximatively given by $-\nabla p\, V$.

Also, viscosity must be considered, since a viscous fluid tend to resist against deforming, i.e. a viscous internal force tries to move a particle to the average of its neighbor particles, which can be measured by the Laplace operator $\Delta = \nabla \cdot \nabla$. Integrating this over V leads approximatively to $\mu \nabla \cdot \nabla \mathbf{u}\, V$ with a dynamic viscosity parameter μ. Adding these terms leads to

$$m\mathcal{D}_t\mathbf{u} = m\mathbf{f} - \nabla p\, V + \mu \nabla \cdot \nabla \mathbf{u}\, V.$$

Navier-Stokes Equation

Assuming a continuous fluid, we can talk the limit such that the particle sizes goes to zero:

$$\mathcal{D}_t \mathbf{u} + \frac{1}{\rho} \nabla p = \mathbf{f} + \nu \nabla \cdot \nabla \mathbf{u}. \tag{3}$$

To understand the concept of the material-derivation operator $\mathcal{D}$, one has to consider Lagrangian and Eulerian viewpoints on a fluid domain, whose connection is expressed by $\mathcal{D}$. In the Lagrangian concept, each point in the fluid domain is labeled as a particle with its own position and velocity.In contrast, from an Eulerian viewpoint, one looks at the fluid from fix grid points in space and observe how its quantities change at these points over time.

For a given quantity $q(\mathbf{x}, t)$, the operator $\mathcal{D}$ is given by its temporal derivative

$$\mathcal{D}_t q := \dot{q}(\mathbf{x}, t) = \partial_t q + \mathbf{u} \cdot \nabla q \tag{4}$$

determined by the chain rule.

Navier-Stokes Equation

Its first part $\partial_t q$ corresponds to an Eulerian measurement which describes the change of q at a fix point $\mathbf{x}$ in space, while the second part $\mathbf{u} \cdot \nabla q$ is a correction to take into account how much of the change is caused by differences in the flow itself.[3]

Substituting an equivalent vector-valued definition of Eq. (4) for the quantity $\mathbf{u}$ into Eq. (3) leads to the Navier-Stokes equation Eq. (1). Its first part

$$\mathcal{D}\mathbf{u} = \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}$$

is mostly denoted as the advection part[4], while the other parts are well-known as pressure part $\nabla p / \rho$, external forces $\mathbf{f}$, and viscosity part $\nu \nabla \cdot \nabla \mathbf{u}$.

[3] To illustrate this, consider a flow which replaces cold with hot air. In this scenario, the change of the temperature in not a result caused by a change of the temperature of a specific molecule.

[4] Equations of the form $\mathcal{D}q = 0$ are usually denoted as advection equations describing the transport through a fluid due to its bulk motion.

Navier-Stokes Equation

In the pressure part, p can be considered as a Lagrange multiplier, which keeps the velocity field divergence free. Taking the divergence of both sides of Eq. (1) and setting

$$\nabla \cdot \partial_t \mathbf{u} = \partial_t \nabla \cdot \mathbf{u} = 0$$

to enforce incompressibility Eq. (2) leads to the pressure equation

$$\nabla \cdot \frac{1}{\rho} \nabla p = \nabla \cdot (\mathbf{f} + \nu \nabla \cdot \nabla \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}).$$

A simple Navier-Stokes solver can be realized by the application of finite differences on Eq. (1).

Euler Equation

More advanced solvers can typically be categorized with respect to the Reynolds number of the simulated scenario. The dimensionless Reynolds number Re describes the ratio of inertia and viscous forces, so that the turbulence behavior of related geometric objects is similar for identical Reynolds numbers.[5]

For non-viscous fluids with a high Reynolds number, the viscosity part can often be ignored, which leads to the so-called Euler equation

$$\mathcal{D}\mathbf{u} + \nabla p/\rho = \mathbf{f}.$$

[5] These numbers are usually defined by $\mathrm{Re} := ud/\nu$ in which u denotes the velocity of the fluid compared to a flowed object and d its characteristic length.

Stokes Flow

In contrast, in the low Reynolds number domain usually corresponding to highly viscous fluids, the advection and pressure parts of Eq. (1) are mostly be ignored, such that the resulting so-called steady Stokes equation becomes linear and can be solved analytically. These equation read

$$\mu \Delta \mathbf{u} = \nabla p - \mathbf{F},$$

in which μ denotes the dynamic viscosity and $\mathbf{F}$ the force. As described in the fundamental work in [Cortez 2001] a regularization can be used in order to realize a suitable integration of these equations. For that, we assume

$$\mathbf{F}(\mathbf{x}) = \mathbf{f}_0 \, \phi_\epsilon(\mathbf{x} - \mathbf{x}_0),$$

in which ϕ_ϵ is a smooth and radially symmetric function with $\int \phi_\epsilon(\mathbf{x}) \, d\mathbf{x} = 1$, spread over a small ball centered at the point $\mathbf{x}_0$.

Stokes Flow

Let G_ϵ be Green's function, i.e. the solution of

$$\Delta G_\epsilon(\mathbf{x}) = \phi_\epsilon(\mathbf{x})$$

and let B_ϵ be the solution of

$$\Delta B_\epsilon(\mathbf{x}) = G_\epsilon(\mathbf{x}),$$

both in the infinite space bounded for small ϵ.

Smooth approximations of G_ϵ and B_ϵ are given by

$$G(\mathbf{x}) = -1/(4\pi \|\mathbf{x}\|)$$

for $\|\mathbf{x}\| > 0$ and

$$B(\mathbf{x}) = -\|\mathbf{x}\|/(8\pi),$$

the solution of the biharmonic equation $\Delta^2 B(\mathbf{x}) = \delta(\mathbf{x})$.

Stokes Flow

The pressure p satisfies $\Delta p = \nabla \cdot \mathbf{F}$, which can be shown by taking the divergence of the steady Stokes equation, and is therefore given by $p = \mathbf{f}_0 \cdot \nabla G_\epsilon$. Using this, we can follow

$$\mu \Delta \mathbf{u} = (\mathbf{f}_0 \cdot \nabla) \nabla G_\epsilon - \mathbf{f}_0 \phi_\epsilon$$

with its solution

$$\mu \mathbf{u}(\mathbf{x}) = (\mathbf{f}_0 \cdot \nabla) \nabla B_\epsilon(\mathbf{x} - \mathbf{x}_0) - \mathbf{f}_0 G_\epsilon(\mathbf{x} - \mathbf{x}_0),$$

the so-called regularized Stokeslet.

Stokes Flow

For multiple forces $\mathbf{f}_1, \ldots, \mathbf{f}_N$ centered at points $\mathbf{x}_1, \ldots, \mathbf{x}_N$, the pressure p and the velocity $\mathbf{u}$ can be computed by superposition. Because G_ϵ and B_ϵ are radially symmetric we can additionally use $\nabla B_\epsilon(\mathbf{x}) = B'_\epsilon \mathbf{x} / \|\mathbf{x}\|$ and get

$$
\begin{aligned}
p(\mathbf{x}) &= \sum_{k=1}^{N} (\mathbf{f}_k \cdot (\mathbf{x} - \mathbf{x}_k)) \frac{G'_\epsilon(\|\mathbf{x} - \mathbf{x}_k\|)}{\|\mathbf{x} - \mathbf{x}_k\|}, \\
\mathbf{u}(\mathbf{x}) &= \frac{1}{\mu} \sum_{k=1}^{N} \Bigg[\mathbf{f}_k \left(\frac{B'_\epsilon(\|\mathbf{x} - \mathbf{x}_k\|)}{\|\mathbf{x} - \mathbf{x}_k\|} - G_\epsilon(\|\mathbf{x} - \mathbf{x}_k\|) \right) \\
&\quad + (\mathbf{f}_k \cdot (\mathbf{x} - \mathbf{x}_k))(\mathbf{x} - \mathbf{x}_k) \frac{\|\mathbf{x} - \mathbf{x}_k\| \, B''_\epsilon(\|\mathbf{x} - \mathbf{x}_k\|) - B'_\epsilon(\|\mathbf{x} - \mathbf{x}_k\|)}{\|\mathbf{x} - \mathbf{x}_k\|^3} \Bigg].
\end{aligned}
$$

Stokes Flow

The flow is satisfies the incompressibility constraint Eq. (2). Since

$$\Delta G_\epsilon(\|\mathbf{x}-\mathbf{x}_k\|) = \frac{1}{\|\mathbf{x}-\mathbf{x}_k\|}(\|\mathbf{x}-\mathbf{x}_k\|\, G_\epsilon'(\|\mathbf{x}-\mathbf{x}_k\|))' = \phi_\epsilon(\|\mathbf{x}-\mathbf{x}_k\|),$$

the integration of

$$G_\epsilon'(\|\mathbf{x}-\mathbf{x}_k\|) = \frac{1}{\|\mathbf{x}-\mathbf{x}_k\|}\int_0^{\|\mathbf{x}-\mathbf{x}_k\|} s\phi_\epsilon(s)\,\mathrm{d}s$$

leads to G_ϵ.

Similarly,

$$\frac{1}{\|\mathbf{x}-\mathbf{x}_k\|}(\|\mathbf{x}-\mathbf{x}_k\|\, B_\epsilon'(\|\mathbf{x}-\mathbf{x}_k\|))' = G_\epsilon(\|\mathbf{x}-\mathbf{x}_k\|)$$

leads to the expression

$$B_\epsilon'(\|\mathbf{x}-\mathbf{x}_k\|) = \frac{1}{\|\mathbf{x}-\mathbf{x}_k\|}\int_0^{\|\mathbf{x}-\mathbf{x}_k\|} sG_\epsilon(s)\,\mathrm{d}s$$

to determine B_ϵ.

Stokes Flow

One can e.g. make use of the specific function

$$\phi_\epsilon(\|\mathbf{x}\|) = \frac{15\epsilon^4}{8\pi(\|\mathbf{x}\|^2+\epsilon^2)^{7/2}},$$

which is smooth and radially symmetric.

Up to now, this allows for the computation of the velocities given the forces. Similarly, one can tread the application of a torque by deriving an analogous so-called regularized rodlet.

In the reverse case, the velocity expressions can be rewritten in the form of the equations

$$\mathbf{u}(\mathbf{x}_i) = \sum_{j=1}^{N} M_{ij}(\mathbf{x}_1,\ldots,\mathbf{x}_N)\mathbf{f}_j$$

for $i \in \{1,\ldots,N\}$ which can be transformed into an equation system $\mathbf{U} = \mathbf{M}\,\mathbf{F}$. Since $\mathbf{M}$ is in general not regular, an iterative solver should be applied.

Level Set Method (LSM)

Given an implicit representation of a $(d-1)$-dimensional curve

$$C := \{\mathbf{x} \in \Omega | \phi(\mathbf{x}) = \text{const.}\}$$

with an embedding function $\phi : \Omega \to \mathbb{R}, \phi(\mathbf{x}) = \text{dist}(\mathbf{x}, C)$ acting on $\Omega \subseteq \mathbb{R}^d$.

We model the temporal evolution of the curve $C(t)$ using a family of embedding functions $\phi(\mathbf{x}, t)$.

According to the definition of C we obtain $\phi(C(t), t)) = \text{const.}$, or equivalently

$$\mathrm{d}_t \phi(C(t), t)) = \nabla\phi \cdot \mathrm{d}_t C + \partial_t \phi = 0.$$

Hamilton-Jacobi Equation (HJE)

This is equivalent to

$$\partial_t \phi = -\nabla \phi \cdot \mathrm{d}_t C.$$

With $\mathrm{d}_t C = F\mathbf{n}$ and outer normal $\mathbf{n} = -\nabla\phi / \|\nabla\phi\|$ we obtain $\partial_t \phi = \nabla\phi \, F \, \nabla\phi / \|\nabla\phi\|$, and finally

$$\partial_t \phi = F \|\nabla\phi\|.$$

For a curve evolution with speed F, the embedding function ϕ must follow according to this so-called Hamilton-Jacobi (level set) equation (HJE).

The speed F typically results from a physical law, see e.g. [Osher Fedkiw 2003], or from a gradient decent procedure in image segmentation, see e.g. [Caselles 1995]'s edge-based geodesic active contours formulating a level set-based snakes approach or [Chan Vese 2010]'s region-based segmentation formulating a level set-based minimization of the Mumford-Shah functional.