

The Structural Method for Partial Differential Equations

Virgile Bertrand^{*,†}, Raphaël Côte^{*}, Victor Michel-Dansac^{*,†}, Emmanuel Franck^{*,†}

^{*} IRMA, Université de Strasbourg, CNRS UMR 7501, 7 rue René Descartes, 67084, Strasbourg, France

[†] Université de Strasbourg, CNRS, Inria, IRMA, F-67000, Strasbourg, France



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- 1 Structural Method
 - From Finite Difference to Structural Method
 - Determining the Structural Equations
 - Handling boundary imposition
 - Generalization to multi-dimensional problems
- 2 Application : Steady-state Stokes Flow
- 3 Conclusion & Perspectives

- 1 **Structural Method**
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- A simple 1D example :

$$\alpha u + \beta \frac{\partial u}{\partial x} + \gamma \frac{\partial^2 u}{\partial x^2} = f \quad \text{on } \Omega =]a, b[\quad (\text{PDE})$$

- FD : Approximate the differential operators evaluated at (inner) points of a mesh $a = x_0 < \dots < x_N = b$. E.g. with a 3 points centered stencil :

$$\left(\frac{\partial u}{\partial x} \right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} \quad , \quad \left(\frac{\partial^2 u}{\partial x^2} \right)_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2}$$

- FD : Puts everything back together, the discretized version of (PDE) becomes :

$$\alpha u_i + \beta \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \gamma \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} = f_i.$$

Structural Method : Separate the Physics & the Discretization

- A simple 1D example :

$$\alpha u + \beta \frac{\partial u}{\partial x} + \gamma \frac{\partial^2 u}{\partial x^2} = f. \quad (\text{PDE})$$

- SM : Introduce state variables for the differential operators evaluated at the mesh points [CLAIN et al. (2023)] :

$$Z_i := u(x_i) \quad D_i := \left. \frac{\partial u}{\partial x} \right|_{x=x_i} \quad S_i := \left. \frac{\partial^2 u}{\partial x^2} \right|_{x=x_i}$$

- SM : The (PDE) can then be rewritten **locally** as :

$$\alpha Z_i + \beta D_i + \gamma S_i = f_i \quad (\text{PE})$$

The Structural Equations (SE)

- Having introduced Z, D, S at each point of the discretized domain, we have to complete the system with **Structural Equations** (SE) in order to solve it
- One could obviously take

$$\frac{Z_{i+1} - Z_{i-1}}{2\Delta x} - D_i = 0 \quad , \quad \frac{Z_{i-1} - 2Z_i + Z_{i+1}}{\Delta x^2} - S_i = 0$$

- And solve the discretized system :

$$\begin{cases} \alpha Z_i + \beta D_i + \gamma S_i = f_i & \text{(PE)} \\ D_i = \frac{Z_{i+1} - Z_{i-1}}{2\Delta x} & \text{(SE1)} \\ S_i = \frac{Z_{i-1} - 2Z_i + Z_{i+1}}{\Delta x^2} & \text{(SE2)} \end{cases}$$

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- More generally, a **Structural Equation** (SE) is a linear combination of the state variables at the stencil points we are considering, e.g. :

$$\sum_{j=i-1}^{i+1} z_j Z_j + d_j D_j + s_j S_j = 0$$

- The question is : how to find some coefficients z_j, d_j, s_j such that the Structural Equation has a high-order of accuracy ?

- If we consider, for $\phi \in \mathcal{C}^2(\mathbb{R})$, the functional :

$$E(\phi) := \sum_{j=i-1}^{i+1} z_j \phi(x_j) + d_j \phi'(x_j) + s_j \phi''(x_j)$$

- Then, if the coefficients z_j, d_j, s_j of our SE satisfies $E(\phi) = 0$ for some ϕ , the SE is exact for ϕ .

→ Choose coefficients such that $E(\phi_k) = 0$ for $\phi_k(x) = (x - x_i)^{k-1}$ for $k = 1, \dots, n$.

Determining the Structural Equations

- Formally, if we consider a polynomial basis $\{\phi_k\}_{k=1}^n$ and $\{(\mathcal{L}_l, s_l)\}_{l=1}^L$ a set of differential operators (associated with a state variable) and some stencil positions, this means that the coefficients $\mathbf{c} \in \mathbb{R}^L$ of the SE are in the kernel of a matrix \mathbf{M} with :

$$(\mathbf{M}_{k,l}) = [\mathcal{L}_l(\phi_k)](x_i + s_l \Delta x)$$

- We can retrieve the FD approximation of $\partial_x u$ with this, indeed :

$$\left(\frac{-1}{2\Delta x}, 0, \frac{1}{2\Delta x}, -1 \right) \in \ker \begin{pmatrix} \phi_k(x_{i-1}) & \phi_k(x_i) & \phi_k(x_{i+1}) & \phi'_k(x_i) \\ 1 & 1 & 1 & 0 \\ -\Delta x & 0 & \Delta x & 1 \\ \Delta x^2 & 0 & \Delta x^2 & 0 \end{pmatrix} \begin{matrix} \phi_1(x)=1 \\ \phi_2(x)=(x-x_i) \\ \phi_3(x)=(x-x_i)^2 \end{matrix}$$

- Note that in 1d, \mathbf{M} is Vandermonde-like, so has a kernel of dimension $L - n$ if $n < L$.

Determining the Structural Equations

- Going back to our example, having introduced Z_i, D_i, S_i we need two Structural Equations in order to close our system.
- We build the matrix \mathbf{M} considering all the state variable on a 3 point centered stencil, and take ϕ_k for $k = 1, \dots, 7$ so that $\dim(\ker \mathbf{M}) = 2$.
- This yields a more intricate scheme of order 6, known as the Combined Compact Scheme [CHU et FAN (1998)] :

$$\left\{ \begin{array}{l} 24 \frac{Z_{i+1} - 2Z_i + Z_{i-1}}{\Delta x^2} - 9 \frac{D_{i+1} - D_{i-1}}{\Delta x} + (S_{i+1} - 8S_i + S_{i-1}) = 0 \\ -15 \frac{Z_{i+1} - Z_{i-1}}{\Delta x^2} + \frac{7D_{i+1} + 16D_i + 7D_{i-1}}{\Delta x} - (S_{i+1} - S_{i-1}) = 0 \end{array} \right. \quad \begin{array}{l} \text{(CSE1)} \\ \text{(CSE2)} \end{array}$$

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- On boundary points, we can introduce the same state variables Z, D, S as in the inner points.
- This allows direct boundary condition imposition, for Dirichlet as well as Neumann, e.g. for a Neumann condition $\frac{\partial u}{\partial x} = g(x)$, we simply impose :

$$D_0 = g(x_{\min}) , D_{N-1} = g(x_{\max})$$

- However we need an extra Structural Equation at the boundary points, indeed the stencil is shifted to the right/left.

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- Direct Generalization : we can simply introduces state variables for partial derivatives in each direction $Z, D_x, D_y, S_{xx}, S_{yy}$ and apply the 1-D SE on each directions. We get a separable problem with a 5-point stencil.
- Multi-dimensional Structural equations : We can determine structural equations with the same recipe as in 1-D, taking for ϕ_k a multi-variate basis of polynomials of degree $\leq N$. However the constructed matrix \mathbf{M} is not Vandermonde-like for $d > 1$.

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Steady-state Stokes Flow

We consider the steady-state Stokes equation in 2D, with $\mathbf{u} = (u, v)$ the velocity field, p the pressure, ν the viscosity and \mathbf{f} a source term :

$$\begin{cases} -\nu\Delta\mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega =]0, 1[^2 \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \end{cases}$$

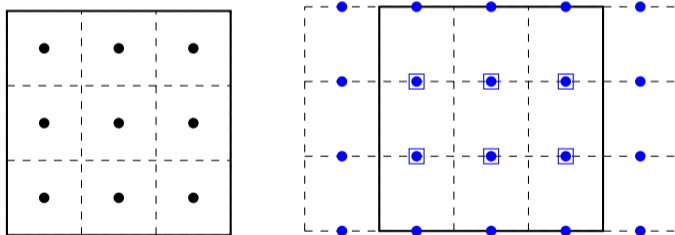


Figure 1 – Location of the variables for the staggered grid. (left) p , $\partial_x u$ and $\partial_y v$ are located at the center of each cell, (right) v as circles, $\partial_y p$, Δv as squares on the mid-point of the horizontal edges.

Steady-state Stokes Flow

Using the presented strategy, we derive a structural equations for the Laplacian by considering a 3×3 stencil for f and a 5-point star stencil for Δf . For the boundary points, the stencil is shifted for the laplacian :

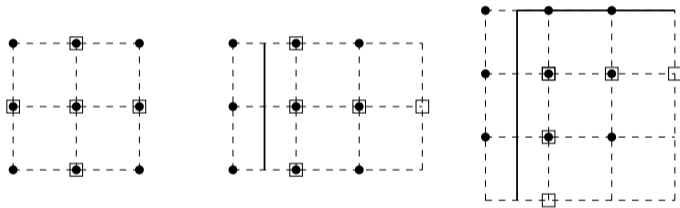


Figure 2 – Stencil for the structural equation for f (circles) and Δf (squares). Left : inner points, middle : points at the left limit of the domain, right : points at the top-left corner of the domain.

Steady-state Stokes Flow

We use a manufactured solution to test the convergence of the method.

$$\begin{cases} \mathbf{u}(x, y) = (\pi \sin(\pi x) \cos(\pi y), -\pi \cos(\pi x) \sin(\pi y)) \\ p(x, y) = \sin(\pi x) \cos(\pi y). \end{cases}$$

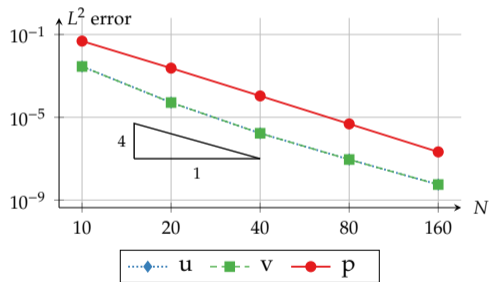
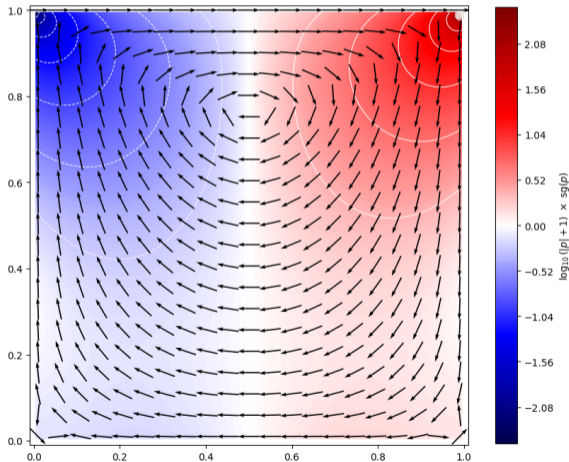


Figure 3 – Convergence of the structural method for the steady-state Stokes flow.

Stokes : Lid-Driven Cavity

If we solve the lid-driven cavity problem, i.e. $u = 1$ on the top boundary and $u = v = 0$ on the other boundaries, we retrieve the expected recirculation pattern :



The Structural Method :

- Gives a clear separation between the physics of the problem (the PDE) and the discretization (the SE).
- Provides a framework to solve PDE on cartesian meshes with high order on compact stencil (and hence good spectral resolution, at least in the 1D case).
- Allow simple boundary condition imposition thanks to the state variables
- As for FD methods, it can be easily implemented, and is especially well suited for PDE with differential operators that depends on the coordinates in the domain (e.g. perfectly matched layers).
- Might be used to impose constraints on the solution that are not guaranteed by the scheme used (e.g. divergence free solutions).
- Easily extendable for non-linear problems, indeed the non-linearity is local to every node of the mesh.

→ at the cost of increased DOFs

- More analysis of the method : stability, spectral properties, etc.
- Adapt the method for discontinuous solutions & shock capturing (e.g. MOOD method).
- Extend the strategy to use it for :
 - Time-dependent PDEs : forward/multistep-stencil.
 - Immersed boundary to handle complex geometries
 - Quad-tree meshes
 - Unstructured meshes - GFDM ?
 - Finite-Volume method ?

- CHU, Peter C. et Chenwu FAN (1998). “A Three-Point Combined Compact Difference Scheme”. In : *Journal of Computational Physics* 140.2, p. 370-399. ISSN : 0021-9991. DOI : <https://doi.org/10.1006/jcph.1998.5899>. URL : <https://www.sciencedirect.com/science/article/pii/S0021999198958995>.
- CLAIN, Stéphane et al. (2023). “Structural schemes for one dimension stationary equations”. In : *Applied Mathematics and Computation* 457, p. 128207. ISSN : 0096-3003. DOI : <https://doi.org/10.1016/j.amc.2023.128207>. URL : <https://www.sciencedirect.com/science/article/pii/S0096300323003764>.