Penguin.jl

A Julia framework for finite-volume PDEs with sharp and moving interfaces

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Roadmap

1. Problem: PDEs with jumps at sharp interfaces
2. Method: cut-cell finite-volume discretization on Cartesian grids
3. Result: sharp interface examples
4. Extension: moving interfaces and phase change problems

Why sharp interfaces for multiphase flows?

Key physics is often localized in a **thin interfacial layer** (μm-nm): phase change, surface reactions, species partitioning, ...

Smearing Γ over a few grid cells [1] leads to:

- effective properties yields closure problem
- phase-dependent physics becomes awkward to impose,
- reduced accuracy overall.

Target

✓ Fixed grid ✓ Sharp jumps at Γ
✓ Conservative

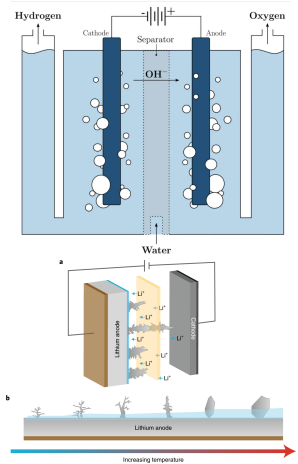


Figure: Electrolysis - Solidification / dendrites

A common sharp-interface template

In each phase $\Omega^{\pm}$:

$$\partial_t \Phi^{\pm} + \nabla \cdot \mathsf{F}^{\pm}(\Phi^{\pm}) = S^{\pm}$$

At the interface Γ:

$$[\![\Phi]\!] = g, \qquad [\![\mathsf{F}\cdot\mathsf{n}]\!] = h$$

Examples in Penguin.jl:

- diffusion - Poisson $\mathsf{F} = -D\nabla\Phi$
- species partitioning $\mathsf{F} = -D\nabla C, \quad [\![C]\!] = (H-1)C^{-}$
- Stokes - Navier-Stokes $\mathsf{F} = -\mu\left(\nabla \mathsf{u} + \nabla \mathsf{u}^{\top}\right) + p\mathsf{I}$
- Stefan - free-boundary $\mathsf{F} = -k\nabla T, \quad h = \rho L\, \mathsf{v}_{\Gamma}\cdot\mathsf{n}$

Numerical question

How do we keep those jumps sharp on a fixed Cartesian grid?

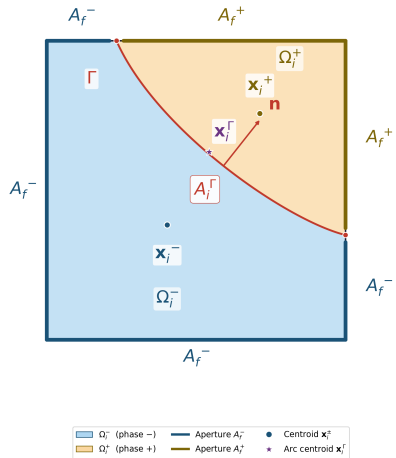
Cut-cell discretization: geometric moments

The interface cuts Cartesian cells. We encode this geometry through **geometric moments**:

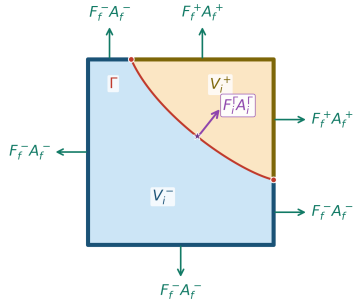
- **phase volumes**: $V_i^{\pm}$
- **open face areas**: $A_f^{\pm}$
- **interface measure**: A_i^{Γ}
- **centroids**: $\mathrm{x}_i^{\pm}$, x_i^{Γ}

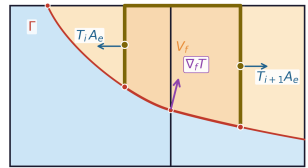
Key point

Only geometric data needed for conservative, compact cut-cell FV operators.



Cut-cell operators + interface DOFs





Finite-volume divergence in phase $\pm$:

$$(\nabla \cdot \mathrm{F})_i \approx \frac{1}{V_i^{\pm}} \left(\sum_f \mathrm{F}_f \cdot \mathrm{n}_f \, A_f^{\pm} + F_i^{\Gamma} A_i^{\Gamma} \right)$$

Gradient on a staggered control volume:

$$\nabla_f T \approx \frac{1}{V_f} \sum_{e \in \partial\Omega_f} T_e \, A_e \, \mathrm{n}_e$$

Introduce interface unknowns $\Phi_i^{\Gamma,\pm}$, one value per side and per cut cell.

One coupled sparse solve

Jump conditions become **additional algebraic equations** for the interface unknowns:

$$\Phi^{\Gamma,+} - \Phi^{\Gamma,-} = g, \qquad F^{\Gamma,+} - F^{\Gamma,-} = A_\Gamma h$$

$$\underbrace{\begin{bmatrix} M_b^- & M_\Gamma^- & & \\ I & & -I & \\ & & M_b^+ & M_\Gamma^+ \\ F_b^- & F_\Gamma^- & F_b^+ & F_\Gamma^+ \end{bmatrix}}_{\mathcal{A}} \begin{bmatrix} \Phi^- \\ \Phi^{\Gamma,-} \\ \Phi^+ \\ \Phi^{\Gamma,+} \end{bmatrix} = \begin{bmatrix} b^- \\ g \\ b^+ \\ A_\Gamma h \end{bmatrix}$$

Payoff

- No penalty parameter
- No ghost cells / extrapolation
- One sparse coupled solve

In Julia, the assembled sparse systems can be solved with `LinearSolve.jl` (direct, Krylov, preconditioned backends).

Henry Mass Transfer across a bubble (2D)

Bulk diffusion in each phase:

$$\partial_t C^{\pm} = \nabla \cdot (D^{\pm} \nabla C^{\pm}) \qquad \text{in } \Omega^{\pm}$$

Henry's law across Γ:

$$[\![C]\!] = (H-1)C^{-}, \qquad [\![D\nabla C \cdot \mathrm{n}]\!] = 0$$

- Sharp Jump amplitude H is **arbitrary**
- **Flux continuity** enforced at the interface
- Second-order accuracy in the bulk

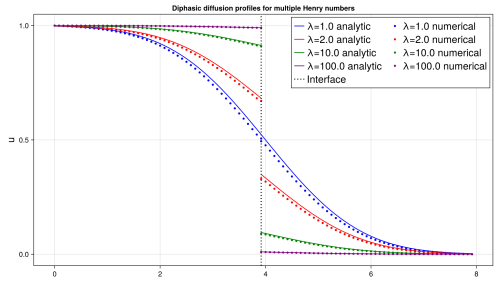
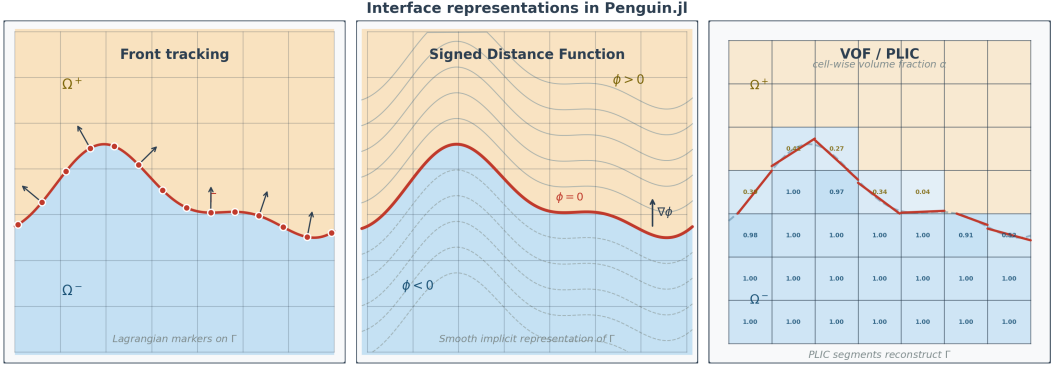


Figure: Radial Concentration profile for various Henry ratios H.

Same cut-cell core, different interface representations

Depending on the physics and topology, Penguin.jl can be coupled to **front tracking**, **signed distance** or **VOF+PLIC** representations.



Moving interfaces: space-time finite volumes

When $\Gamma(t)$ moves, cells can **appear** or **disappear**.

Classical fixes

- Extrapolation: non-conservative
- Cell merging: ad hoc
- Redistribution: only global conservation

Space-time finite volume

Extrude cells over $[t^n, t^{n+1}]$: interface motion becomes a cut in **space-time**.
Fresh / dead cells are simply space-time cut cells.

Local conservation and GCL hold by construction.

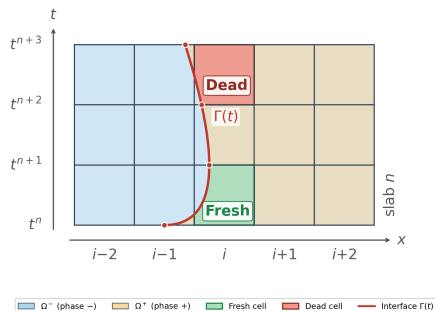


Figure: Space-time control volumes.

Moving interface example: Deforming bubble

Concentration C across a **prescribed moving interface**:

$$\partial_t C^{\pm} = \nabla \cdot (D^{\pm} \nabla C^{\pm}) \qquad \text{in } \Omega^{\pm}(t)$$

- Space-time cut cells handle **fresh/dead cells** automatically
- Jump $[\![C]\!]$ enforced at each time step
- **Local conservation** holds by construction (GCL)
- What if the interface motion depends on the solution?

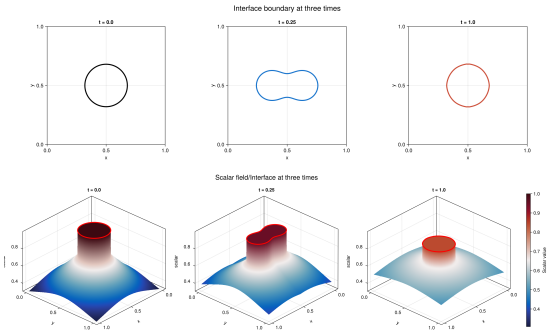
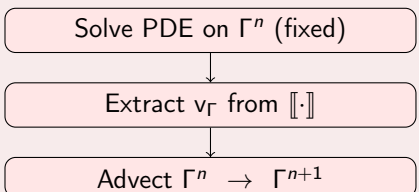


Figure: Concentration field around a moving bubble.

Free boundaries: coupled solve beats splitting

Splitting (classical)



Problem: geometry changes *after* the solve.
Solved domain $\neq$ final domain.

Coupled solve (Penguin.jl)

Find Φ^{n+1} *and* Γ^{n+1} simultaneously:

$$\begin{cases} \mathcal{L}(\Phi^{n+1}, \Gamma^{n+1}) = 0 & \text{(bulk PDE)} \\ \mathcal{R}(\Phi^{n+1}, \Gamma^{n+1}) = 0 & \text{(jump cond.)} \end{cases}$$

Inner loop per time step:

1. Fix $\Gamma^{(k)}$, solve bulk PDE $\rightarrow \Phi^{(k)}$
2. Compute residual $\mathcal{R}(\Phi^{(k)}, \Gamma^{(k)})$
3. Update $\Gamma^{(k+1)}$ to reduce residual
4. Repeat until $|\mathcal{R}| \approx \varepsilon_{\text{mach}}$

Coupled Stefan iterations converge rapidly

- **1st iteration**: classical advection algorithm
- **Next iterations**: inner corrections
- **3-10 iterations** usually enough
- Final residual at **machine precision**

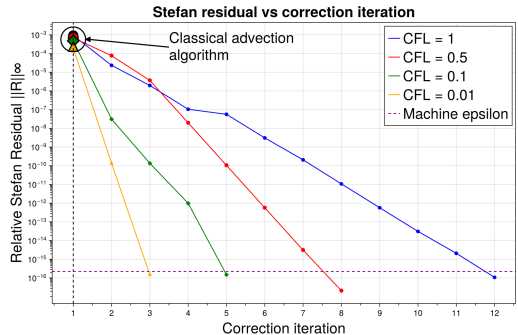


Figure: Fast residual decay of the Stefan correction loop.

Phase change (Stefan) and dendrites

Energy jump drives interface velocity:

$$[\![k\nabla T\cdot \mathrm{n}]\!] = \rho L\, \mathrm{v}_\Gamma \cdot \mathrm{n}$$

Observations:

- Planar fronts converge at **second order** (appendix)
- Unstable modes match Mullins-Sekerka [4]
- Full **dendrite patterns** without ad hoc fixes

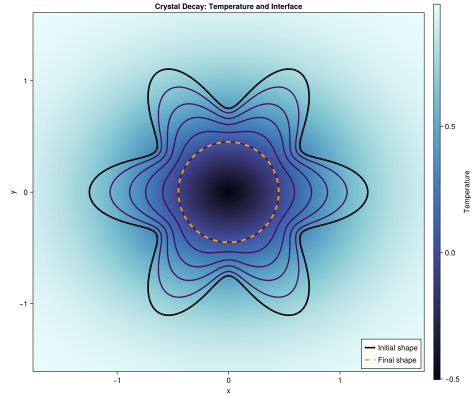
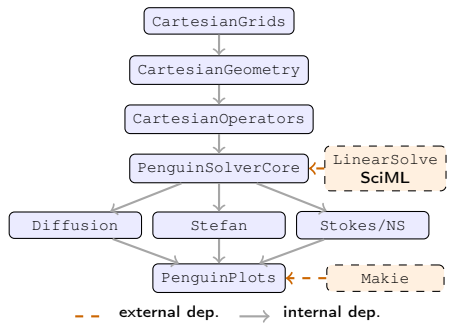


Figure: Dendritic growth: temperature field and tracked interface.

Why Julia for Penguin.jl?

- **Multiple dispatch**: the same `grad/div` work with front tracking, SDF, or VOF
- **Composable packages**: geometry, operators, and physics solvers share one core
- **SciML interoperability**: `LinearSolve.jl` gives direct and iterative backends
- **One-language workflow**: geometry, discretization, and solvers all in Julia



One Julia workflow: coupled Stefan / free boundary

```
using CartesianGeometry, PenguinBCs, PenguinStefan

# geometry from a front-tracking interface
grid  = (0.0:0.1:1.0, 0.0:0.1:1.0)
ft_circle = sample_circle(...)

# outer boundary conditions
bc = BorderConditions(; left=Dirichlet(...), right=Dirichlet(...))

# interface representation + Stefan problem
rep  = FrontTrackingRep(grid, ft_circle; coupling = :ft_lm, max_iter = ...)
# rep = LevelSetRep(...)
prob = StefanDiphProblem(..., rep; bc_border = bc)

# build and march the coupled solver
solver = build_solver(prob; t0 = 0.0, uω0 = uω0, uγ0 = uγ0)
solve!(solver, (0.0, t_end); dt = Δt)
```

Takeaways & next steps

What to remember

- **Two-fluid** + cut cells: sharp jumps on a Cartesian grid
- **Operators** built from geometric moments
- **Interface DOFs**: enforce jumps directly
- **Space-time FV**: moving interfaces with local conservation
- **Strong coupling**: free boundaries without splitting error

Next steps

- 3D space-time (4D cut cells)
- NS + species + Stefan coupling
- **Parallelisation**: via `MPI.jl`: non-linear iterations and implicit solves are the bottleneck
- **GPU port** via `KernelAbstractions.jl`: backend-agnostic kernels for FV operators

Thank you - Questions?

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Towards a sharp, structure preserving two-velocity model for two-phase flow: transport of mass and momentum.
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Stability of a planar interface during solidification of a dilute binary alloy.
Journal of Applied Physics, 35(2):444-451, 1964.

Two-phase Poisson equation: Julia 3-circle logo

$$-\nabla\cdot\left(\beta^{\pm}\nabla\Phi^{\pm}\right) = f^{\pm} \qquad \text{in } \Omega^{\pm}$$

Sharp interface conditions on Γ:

$$[\![\Phi]\!] = g(\mathrm{x}), \qquad [\![\beta\nabla\Phi\cdot\mathrm{n}]\!] = h(\mathrm{x})$$

- Multiple disconnected interfaces handled in one solve
- Sharp jump captured without smearing
- Clean error localization near Γ

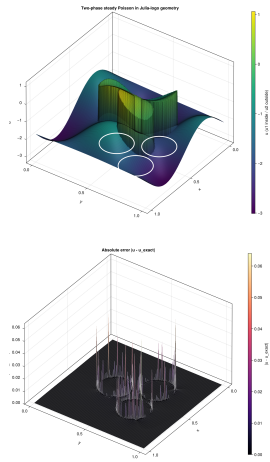

Figure: Top: solution. Bottom: error.

Appendix - Henry jump: gain over one-fluid

n	Cut-cell error	One-fluid error	Improvement
1	3.06×10^{-1}	-	$\times 1.0$
2	6.69×10^{-3}	1.59×10^{-2}	$\times 2.4$
4	1.36×10^{-3}	9.85×10^{-3}	$\times 7.2$
8	3.24×10^{-4}	5.45×10^{-3}	$\times 16.8$
16	5.25×10^{-5}	2.75×10^{-3}	$\times 52.5$
32	6.46×10^{-6}	1.42×10^{-3}	$\times 220$
64	1.26×10^{-6}	7.03×10^{-4}	$\times 560$
128	1.94×10^{-7}	3.32×10^{-4}	$\times 1707$
Observed order	2.56	1.1	-

- Sharp cut-cell is already solvable at $n = 1$
- Only **one cell inside the bubble**
- Gain increases strongly with refinement

Appendix - Static sharp-interface diffusion

```
using CartesianGeometry, CartesianOperators, PenguinBCs, PenguinDiffusion

# geometry in each phase
body(x, y) = ...
moms1 = geometric_moments( body, grid, Float64, nan; method = :vofijul)
moms2 = geometric_moments(-body, grid, Float64, nan; method = :vofijul)

# outer BCs + interface jump conditions
bc = BorderConditions(; left=Dirichlet(...), right=Dirichlet(...))
ic = InterfaceConditions(
    scalar = RobinJump(α, β, g),
    flux   = FluxJump(1.0, 1.0, 0.0))

# cut-cell operators and diphasic model
cap1, cap2 = assembled_capacity(moms1), ...
ops1, ops2 = DiffusionOps(cap1; periodic = periodic_flags(bc, 2)), ...

model = DiffusionModelDiph(cap1, ops1, D1, s1, cap2, ops2, D2, s2;
                           bc_border = bc, ic = ic)
sol = solve_steady!(model)
```

Appendix - Stefan front accuracy

h ($\Delta t = 0.5h$)	$\|T - T_{\text{exact}}\|_2$	$\|s - s_{\text{exact}}\|$	avg iters	last iters
0.2	1.82×10^{-2}	5.69×10^{-3}	24.25	18
0.1	4.84×10^{-3}	1.65×10^{-3}	24.63	14
0.05	1.44×10^{-3}	5.40×10^{-4}	18.27	12
0.025	3.58×10^{-4}	1.47×10^{-4}	14.47	11
0.0125	8.76×10^{-5}	3.42×10^{-5}	11.92	10
0.00625	2.56×10^{-5}	8.70×10^{-6}	10.06	9
0.003125	1.12×10^{-5}	1.92×10^{-6}	8.67	6
Observed order	1.83	1.92	-	-

- Nearly second-order convergence for both temperature and interface position
- Inner correction count decreases with mesh refinement
- Final correction step typically needs only 6-18 iterations

Appendix - FT least-squares correction

Predict a front $\Gamma^{n+1}_{\text{pred}}$, then correct it by normal displacements

$$x_v(d) = x_{v,\text{pred}} + d_v \, n_v^{\text{pred}}.$$

For each candidate front:

$$\Gamma^{n+1}(d) \;\longrightarrow\; \text{space-time diffusion solve} \;\longrightarrow\; r(d) \;\longrightarrow\; \min_d \; \mathcal{J}(d)$$

with

$$r_i(d) = \rho L\big(V_i^{n+1}(d) - V_i^n\big) + \Phi_i(d), \qquad \mathcal{J}(d) = \tfrac{1}{2}\|W\, r(d)\|_2^2 + \tfrac{1}{2} d^\top R d.$$

- near-2nd-order recovered for temperature and interface position
- average inner iterations decrease with refinement
- **1 iteration** typically reduces the residual by a factor 5-20

Appendix - Cut-cell incompressible flow

In each phase:

$$\rho^{\pm}\left(\partial_t \mathsf{u}^{\pm} + \mathsf{u}^{\pm}\cdot\nabla\mathsf{u}^{\pm}\right) = -\nabla p^{\pm} + \nabla\cdot\left(2\mu^{\pm}\mathsf{D}(\mathsf{u}^{\pm})\right) + \mathsf{f}^{\pm}$$

$$\nabla\cdot\mathsf{u}^{\pm} = 0$$

Across the sharp interface Γ:

$$[\![\mathsf{u}]\!] = 0, \qquad [\![\boldsymbol{\sigma}\mathsf{n}]\!] = \mathsf{t}_\Gamma$$

$$\boldsymbol{\sigma} = -p\,\mathsf{I} + 2\mu\mathsf{D}(\mathsf{u}), \qquad \mathsf{D}(\mathsf{u}) = \tfrac{1}{2}\left(\nabla\mathsf{u} + \nabla\mathsf{u}^{\top}\right)$$

- Same cut-cell / staggered-grid philosophy
- Sharp velocity and traction conditions at Γ

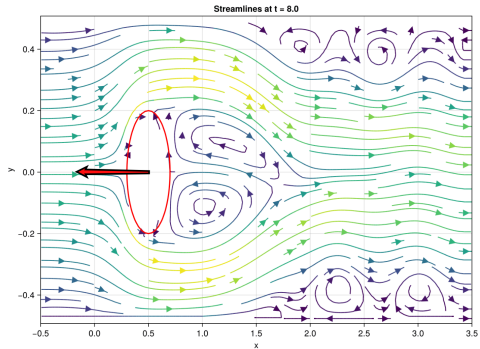

Figure: Representative incompressible-flow example on a Cartesian cut-cell grid.