A volume-preserving semi-Lagrangian trajectory scheme

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•Semi-Lagrangian schemes arise from a path integration

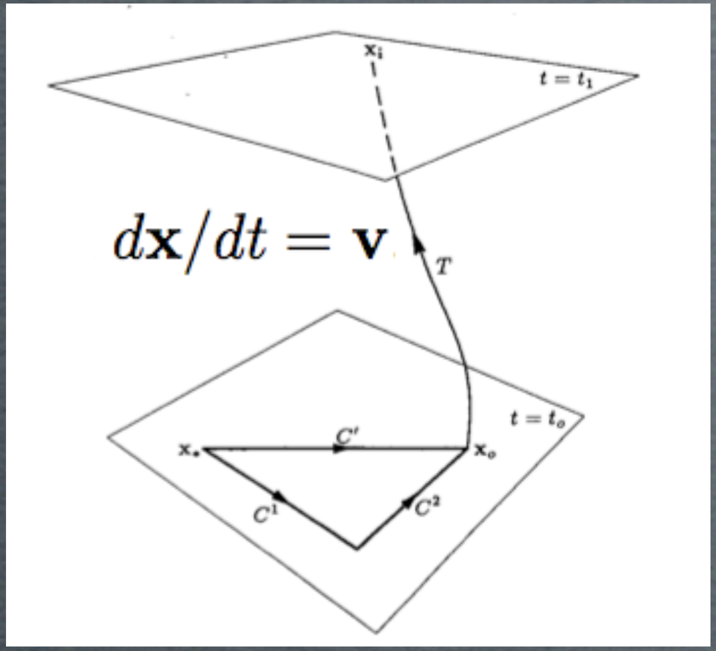
arrival point

$$\psi(\mathbf{x},t)=\psi(\mathbf{x}_0,t_0)+\int_T R\,d\,t$$

departure point

of the corresponding Lagrangian evolution equation: $\frac{d\,\psi}{d\,t}=R$

For instance, in MHD: $\frac{d\mathbf{\Psi}}{dt}=\mathbf{R}$ $\quad \mathbf{\Psi}=\{\mathbf{u},\Theta',\mathbf{B}\}^T$ $\quad \mathbf{R}=\{\mathbf{R}_\mathbf{u},R_{\Theta'},\mathbf{R}_\mathbf{B}\}^T$



(1) Find $(\mathbf{x}_0,t_0)$: $\mathbf{x}_0=\mathbf{x}_\mathbf{i}-\int_{t_0}^{t}\mathbf{v}(\mathbf{x}(\tau),s)d\,s$

(2) $\psi(\mathbf{x}_\mathbf{i},t_0)\rightarrow\psi(\mathbf{x}_0,t_0)$ (interp.)

EULAG template algorithm:

(3): $\psi_\mathbf{i}^{n+1}=LE_\mathbf{i}(\tilde{\psi})+0.5\Delta t R_\mathbf{i}^{n+1}\;\equiv\;\widehat{\psi}_\mathbf{i}+0.5\Delta t R_\mathbf{i}^{n+1}$

•We are interested in the *compatibility* of step (1) with the fundamental equations of fluid dynamics.

- The *flow Jacobian* is the ratio of infinitesimal volumes of a fluid element before and after transport of that element: $\mathrm{J} := \det(\partial \mathbf{x}/\partial \mathbf{x}_0)$ and its evolution is governed by the fundamental Euler expansion

$$\frac{d \ln \mathrm{J}}{dt} = \nabla \cdot \mathbf{v}$$

- Thus, vortical motion does not change the volume of a fluid element. Indeed, $\mathbf{v} = \nabla \boldsymbol{\Psi} + \nabla \times \mathbf{A}$ (Stokes decomposition) $\longrightarrow$ $\nabla \cdot \mathbf{v} = \nabla \cdot (\nabla \boldsymbol{\Psi}) + \underbrace{\nabla \cdot (\nabla \times \mathbf{A})}_{=0}$

- The simplest case is that of incompressible fluids, the only one we shall consider here.

- Now, a standard trajectory estimate has the form

$$\mathbf{x}_0 = \mathbf{x}_\mathrm{i} - \int_{t_0}^{t} \mathbf{v}(\mathbf{x}(\tau), s)\, d\, s \longrightarrow \tilde{\mathbf{x}}_0 \approx \mathbf{x}_\mathrm{i} - \Delta t \tilde{\mathbf{v}}$$

(e.g. for Euler Forward $\mathbf{v} = \tilde{\mathbf{v}}$)

↑ "path-mean velocity"

- Correct for the part of the path-mean velocity that *causes* changes in the volume $\longrightarrow$ $(\tilde{\mathbf{x}}_0)_C = \mathbf{x}_\mathrm{i} - \Delta t \left(\tilde{\mathbf{v}} - \nabla \phi\right)$

•Combining the mass continuity equation and the Euler expansion formula leads to the Lagrangian form of the mass continuity:

$$\frac{d\rho}{dt} = -\rho\nabla\cdot\mathbf{v} \quad + \quad \frac{d\ln \mathrm{J}}{dt} = \nabla\cdot\mathbf{v} \quad \rightarrow \quad \rho(\mathbf{x}_\mathrm{i}, t) = \widehat{\mathrm{J}}\rho(\mathbf{x}_0, t_0)$$

*

$$\widehat{\mathrm{J}} \equiv \mathrm{J}^{-1} = \det(\partial\mathbf{x}_0/\partial\mathbf{x})$$

•Now $\nabla\cdot\mathbf{v} = 0$, and so this implies $\mathrm{J} = 1$.

•However, errors in the trajectory estimates can result in the violation of the *compatibility* of the integrals of motion with *

•Therefore, $\widehat{\mathrm{J}} = 1$ is called the *compatibility condition.*

•Substituting the expression for the correction $(\tilde{\mathbf{x}}_0)_C = \mathbf{x_i} - \Delta t \left(\tilde{\mathbf{v}} - \nabla\phi\right)$ into the compatibility condition $\widehat{\mathrm{J}} = 1$ gives rise to a second order non-linear PDE:

$$\det\left\{\frac{\partial(\tilde{\mathbf{x}}_0)_C}{\partial \mathbf{x}}\right\} = 1$$

,

The Monge-Ampère equation(MAE).

•Found in mathematical physics, differential geometry, optimization (e.g. MKP), image registration (e.g. medical imagery), cosmology (reconstructing early universe) and fluid dynamics.

•For instance, in 2D it takes the form

$$A\phi_{xx} + 2B\phi_{xy} + C\phi_{yy} + E(\phi_{xx}\phi_{yy} - \phi_{xy}^2) + D = 0$$

•Coefficients are functions of the velocity derivatives, and thus of strain/rotation tensor entries.

Some properties-1

•Ellipticity : "A nonlinear PDE is elliptic at a solution Φ_0 if its linearization is elliptic at Φ_0. (mathworld)

$$\Phi = \Phi_0 + \epsilon\widehat{\Phi} \rightarrow \widehat{\Phi}_{xx}(A + E\Phi_{0yy}) + 2\widehat{\Phi}_{xy}(B - E\Phi_{0xy}) + \widehat{\Phi}_{yy}(C + E\Phi_{0xx}) = 0$$

$$\epsilon \lll 1$$

$$\rightarrow \quad \Delta = (A + E\Phi_{0yy})(C + E\Phi_{0xx}) - (B - E\Phi_{0xy}) = AC - B^2 - DE$$

$$\rightarrow \quad AC - B^2 - DE > 0 \leftrightarrow \mathrm{L} := \Delta t \left\| \frac{\partial \tilde{\mathbf{v}}}{\partial \mathbf{x}} \right\| < 1$$

The "Lipschitz number" controls confluence/divergence of the estimated flow trajectories (Smolarkiewicz & Pudykiewicz, JATM1992)

•Prevents trajectories from intersecting one another.

•Necessary condition for convergence of the MA solver.

Numerical approach

- Compute backward trajectory estimates

$$\mathbf{x}_0^0 \equiv \mathbf{x_i} - \Delta t \mathbf{v}(\mathbf{x_i}, t)$$

$$\mathbf{x}_0^\nu = \mathbf{x_i} - \frac{1}{2}\Delta t(\mathbf{v}(\mathbf{x}_0^{\nu-1}, t_0) + \mathbf{v}(\mathbf{x_i}, t)) \quad , \ \nu = 1, \dots, m$$

- Formulate the BVP using a functional form

$$(\tilde{\mathbf{x}}_0)_C = \mathbf{x}_0^m + \Delta t \nabla \phi \quad , \ m = 0, 1, 2, \dots \ . \longrightarrow F(\phi) \equiv \det\left\{\frac{\partial(\mathbf{x}_0)_C}{\partial \mathbf{x}}\right\} - 1 = 0$$

- Use few steps of a Newton-Krylov solver

$$F(\phi^{n+1}) = F(\phi^n) + F'(\phi^n)(\phi^{n+1} - \phi^n) + \text{H.O.T.} \longrightarrow F(\phi^{n+1}) = 0$$

$$F'(\phi^n)\xi = -F(\phi^n) \qquad \xi := \phi^{n+1} - \phi^n$$

- An approximate linearized solution is found using kth order GCR

$$\frac{\partial^k \mathcal{P}(\xi)}{\partial \tau^k} + \frac{1}{T_{k-1}}\frac{\partial^{k-1}\mathcal{P}(\xi)}{\partial \tau^{k-1}} + \dots + \frac{1}{T_1}\frac{\partial \mathcal{P}(\xi)}{\partial \tau} = \mathcal{R}(\xi) \qquad \mathcal{R}(\xi) = F'(\phi^n)\xi + F(\phi^n)$$

- Works for linear non-symmetric elliptic operator

Some properties of solutions

Unicity of solutions and the Rellich theorem (Rellich, 1933) :
Given that the MAE is elliptic, there is at most one solution for which

$$E\phi_{xx} + C > 0 \;, E\phi_{yy} + A > 0$$ type-1

and at most one for which

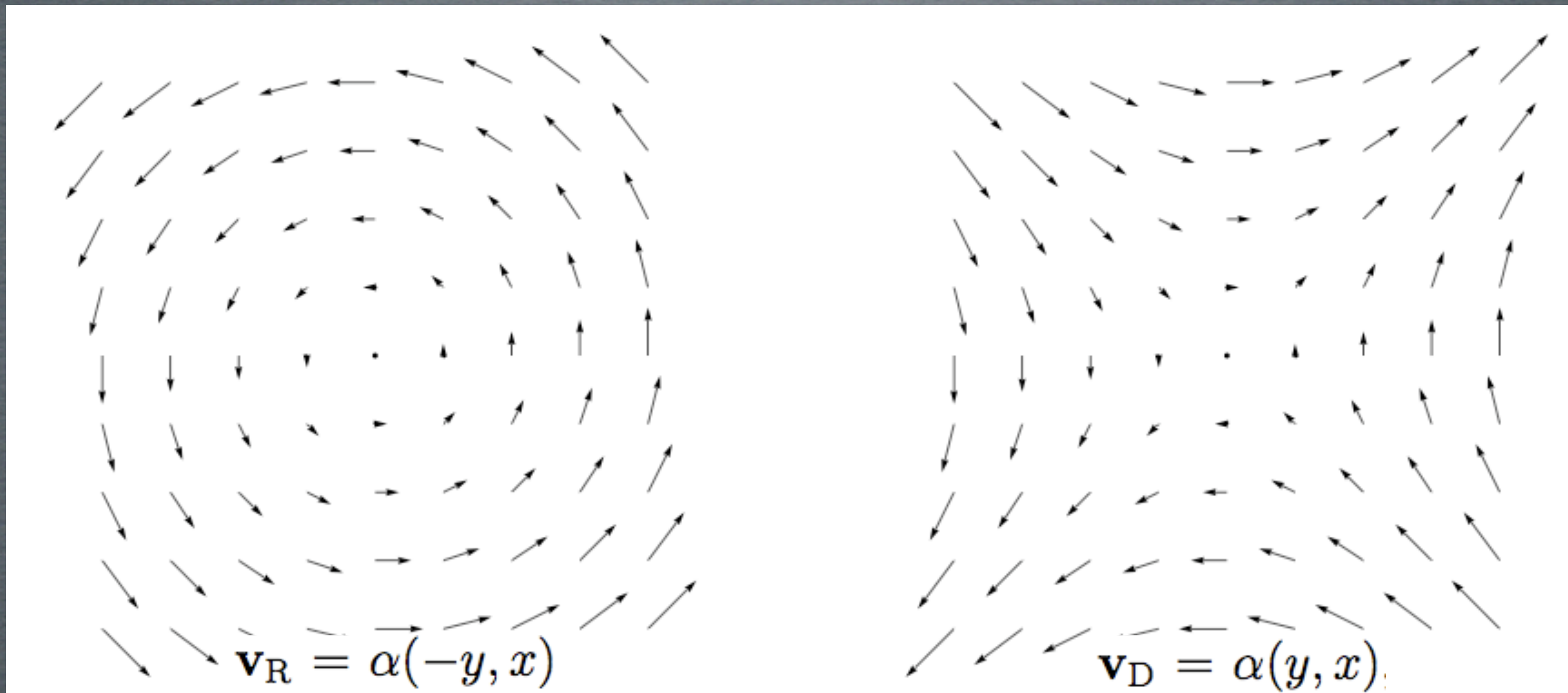
$$E\phi_{xx} + C < 0 \;, E\phi_{yy} + A < 0 \;,$$ type-2

given that they share the same boundary conditions. (Courant & Hilbert)

Based on this theorem, there can be at most two solutions to the MAE for given coefficients and boundary conditions.

Solutions that satisfy the first and second conditions shall be referred to as type-1 and type-2 solutions.

Elemental flow theory-1



$\mathbf{v}_\mathrm{R} \longrightarrow (\Omega_{12} = -\Omega_{21} = -\alpha,\ \Omega_{11} = \Omega_{22} = 0,\ \mathbf{D} = 0)$:pure rotation

$\mathbf{v}_\mathrm{D} \longrightarrow (D_{12} = D_{21} = \alpha,\ D_{11} = D_{22} = 0,\ \mathbf{\Omega} = 0)$:pure deformation

Elemental flow theory-2

- We seek an exact solution for the case of pure rotation

$\mathbf{v}_\mathrm{R} \longrightarrow$ $\phi_{xx} + \phi_{yy} + \Delta t(\phi_{xx}\phi_{yy} - \phi_{xy}^2) + \alpha^2 \Delta t = 0$

flow symmetry: Reduction to a 2nd ord. nonlin. ODE

$F(\xi) = F(x^2 + y^2)$ $\longrightarrow$ $4F_\xi(1 + \Delta t F_\xi) + 4\xi F_{\xi\xi} + 8\Delta t \xi F_\xi F_{\xi\xi} + \alpha^2 \Delta t = 0$

- The general solution is given by

$$F = \frac{-\xi}{2\Delta t}\left(1 \mp \left(\beta^2 + \frac{\exp(C_1)}{\xi}\right)^{1/2}\right) \pm \frac{\exp(C_1)}{4\beta\Delta t} \log\left[\exp(C_1) + 2\beta\xi\left\{\beta + \left(\beta^2 + \frac{\exp(C_1)}{\xi}\right)^{1/2}\right\}\right] + C_2 \ ,$$

- The MAE is elliptic provided that $AC - B^2 - DE = \beta^2 = 1 - \alpha^2 \Delta t^2 > 0$.

- C_1 sets the value of the derivatives on a circle $\xi = x^2 + y^2 = \mathrm{cst}$

$\longrightarrow$ $\nabla\phi|_{(0,0)} = 0$ $\longrightarrow$ $C_1 \to -\infty$ $\longrightarrow$ $F = -\frac{\xi}{2\Delta t}(1 \pm \beta)$

Elemental flow theory-3

- Unicity: Applying the Rellich theorem gives

$$E\phi_{xx} + C = \Delta t\phi_{xx} + 1 > 0, \quad E\phi_{yy} + A = \Delta t\phi_{yy} + 1 > 0$$

for type-1 solutions and

$$E\phi_{xx} + C = \Delta t\phi_{yy} + 1 < 0, \quad E\phi_{yy} + A = \Delta t\phi_{yy} + 1 < 0$$

for type-2 solutions.

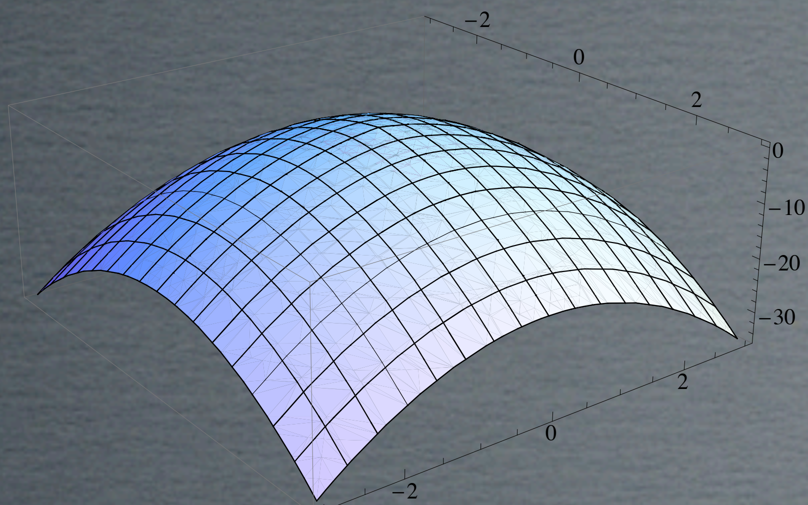
Let's check:

$$F_{xx} = -\frac{1}{\Delta t} \pm \frac{1}{\Delta t}\left(y^2\xi^{-2}\exp(C_1) + \beta^2\right)\left(\beta^2 + \frac{\exp(C_1)}{\xi}\right)^{-1/2}$$

Therefore we have: $F_{xx}(+) > -1/\Delta t$ and $F_{xx}(-) < -1/\Delta t$

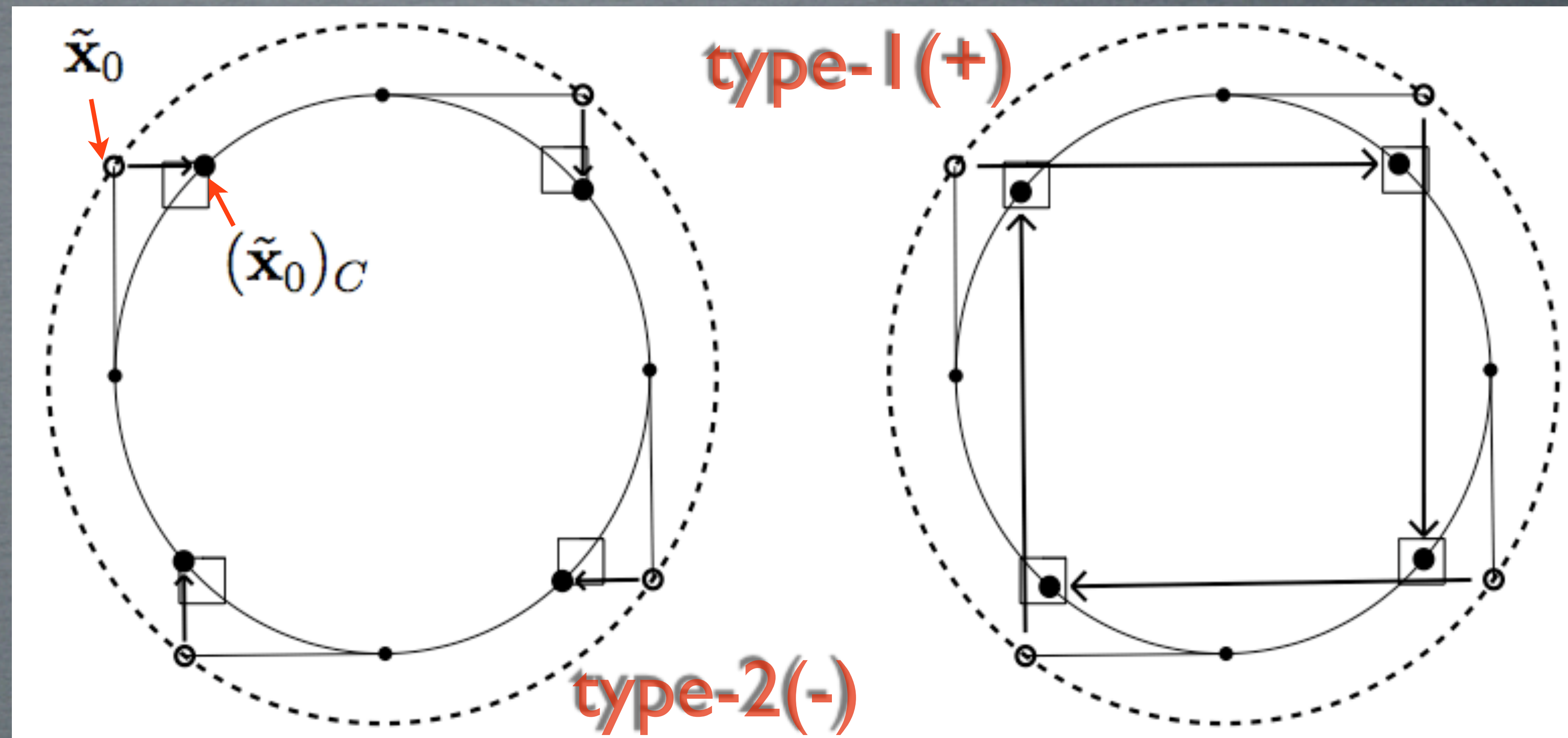
Thus, $F(+)$ and $F(-)$ qualify as type-1 and type-2 solutions.

Elemental flow theory-5



$$F = -\frac{\xi}{2\Delta t}(1 \pm \beta)$$

$$(\tilde{\mathbf{x}}_0)_C = \mathbf{x_i} - \Delta t(\tilde{\mathbf{v}} - F_\xi \nabla \xi)$$



- Both solutions produce volume-preserving sets of departure points.
- Type-2 is closer to the exact trajectory that type-1: solver convergence
- A MAE solution that provides the set of exact departure points does not exist

$$e_x = x - \Delta t(-\alpha y) - (x\cos(\alpha\Delta t) + y\sin(\alpha\Delta t))$$
$$e_y = y - \Delta t(\alpha x) - (-x\sin(\alpha\Delta t) + y\cos(\alpha\Delta t))$$

$$\text{error} = \nabla\Psi + \nabla \times \mathbf{A}$$

$$\nabla \times \mathbf{e}_R = \hat{\mathbf{z}}(\partial_x e_y - \partial_y e_x) = 2\hat{\mathbf{z}}(\alpha\Delta t + \sin\alpha\Delta t) \neq 0 \text{ for } \Delta t > 0.$$

Elemental flow theory-6

$\mathbf{v}_{\mathrm{D}} \longrightarrow$ $$\phi_{xx} + \Delta t \phi_{xy} + \phi_{yy} + \Delta t(\phi_{xx}\phi_{yy} - \phi_{xy}^2) - \alpha^2 \Delta t = 0$$

- Always elliptic.
- No obvious symmetries: let's try to find solutions that would provide us with the exact departure points, i.e. solve:

$$\mathbf{x}_0 - \mathbf{x}_{\mathrm{i}} + \Delta t(\mathbf{v} - \nabla \phi) = 0$$

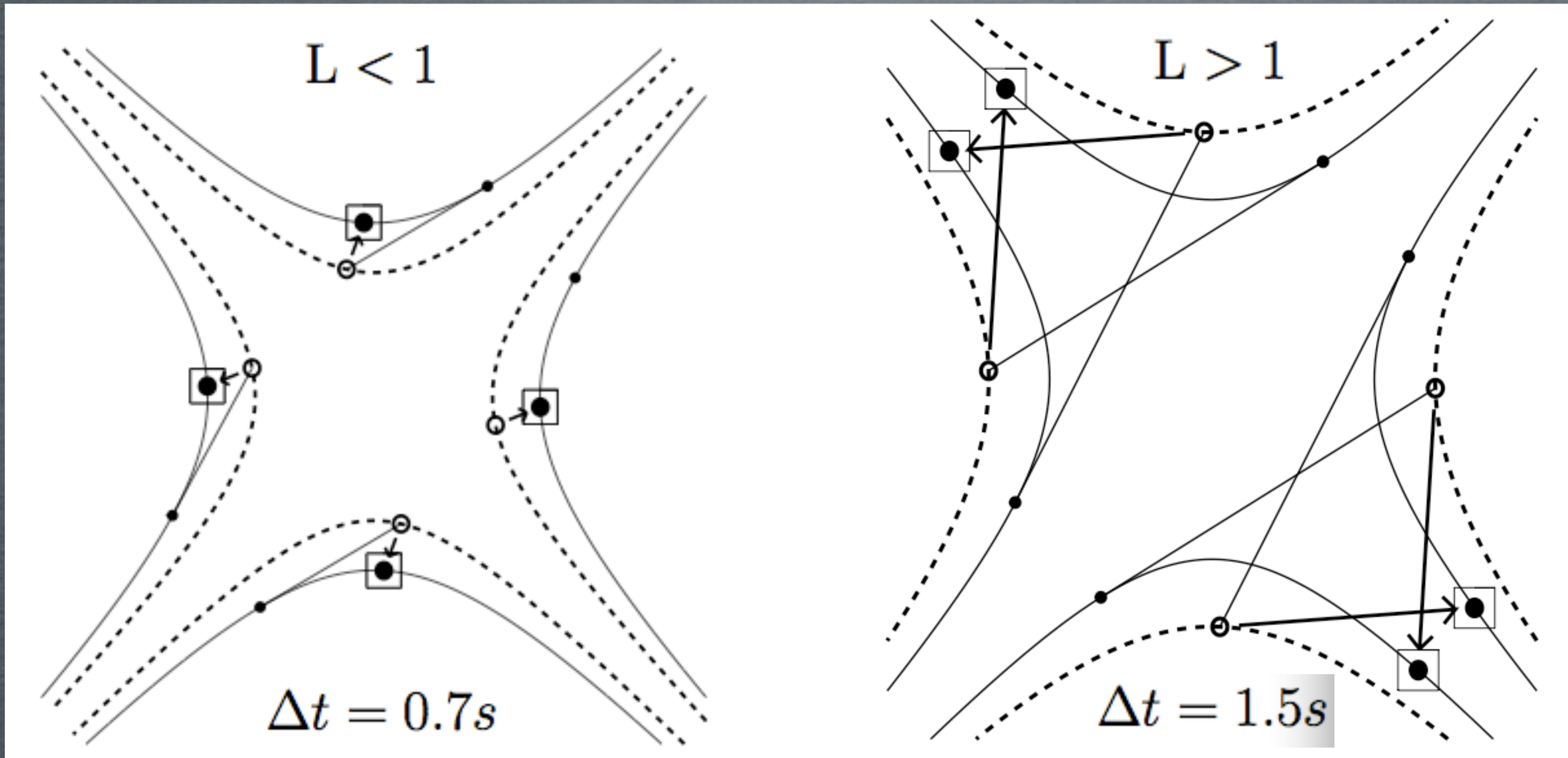
$$\phi := \left(\frac{x^2 + y^2}{2\Delta t}\right)(\cosh(\alpha \Delta t) - 1) - \frac{xy}{\Delta t}(\sinh(\alpha \Delta t) - \alpha \Delta t)$$

- Substituting the latter into the MAE proves that it is a viable solution. Unlike the case of pure rotation, the numerical error does not have a vortical part, and the MAE correction is able to fully take it into account.

$$\text{error} = \nabla \Psi + \nabla \times \mathbf{A}$$

0

Elemental flow theory-7



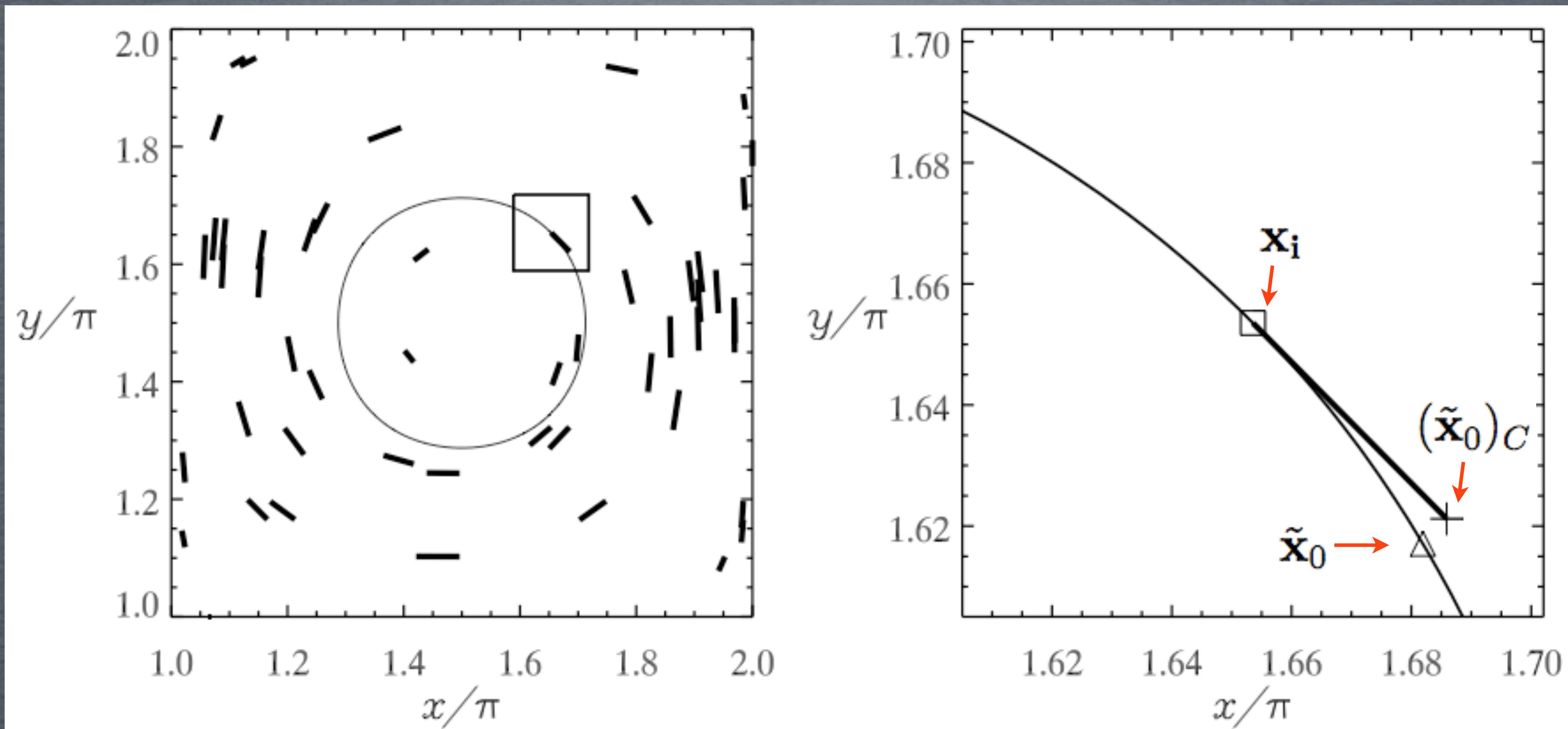
- Lipschitz number: sufficient but not necessary condition for ellipticity of the MAE.

$$e_x = x - \Delta t(\alpha y) - (x\cosh(\alpha\Delta t) - y\sinh(\alpha\Delta t))$$
$$e_y = y - \Delta t(\alpha x) - (-x\sinh(\alpha\Delta t) + y\cosh(\alpha\Delta t))$$

$$\longrightarrow \quad \nabla \times \mathbf{e}_D = 0$$

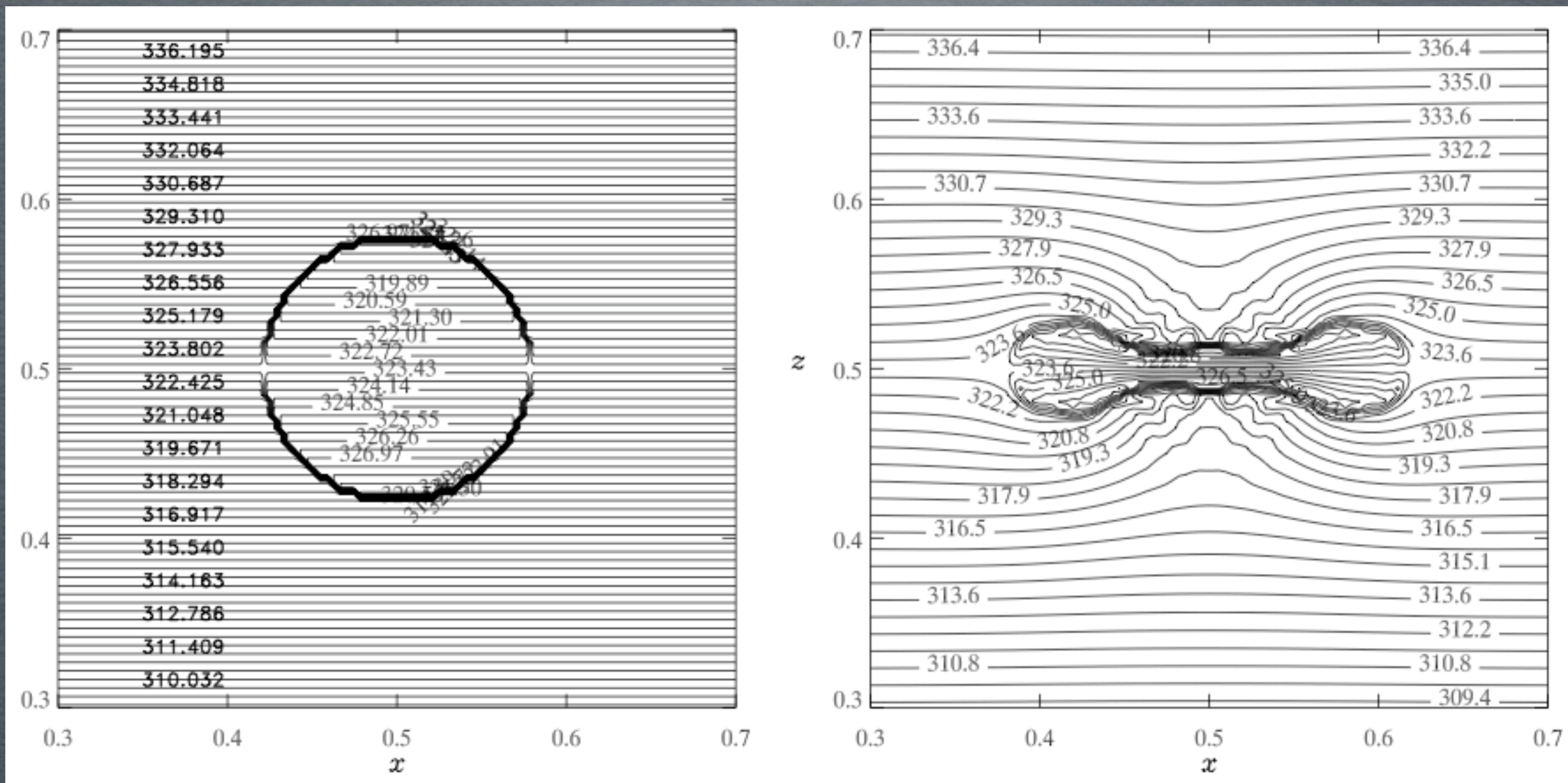
A numerical example

stream-function $\zeta = \sin(x)\sin(y)$



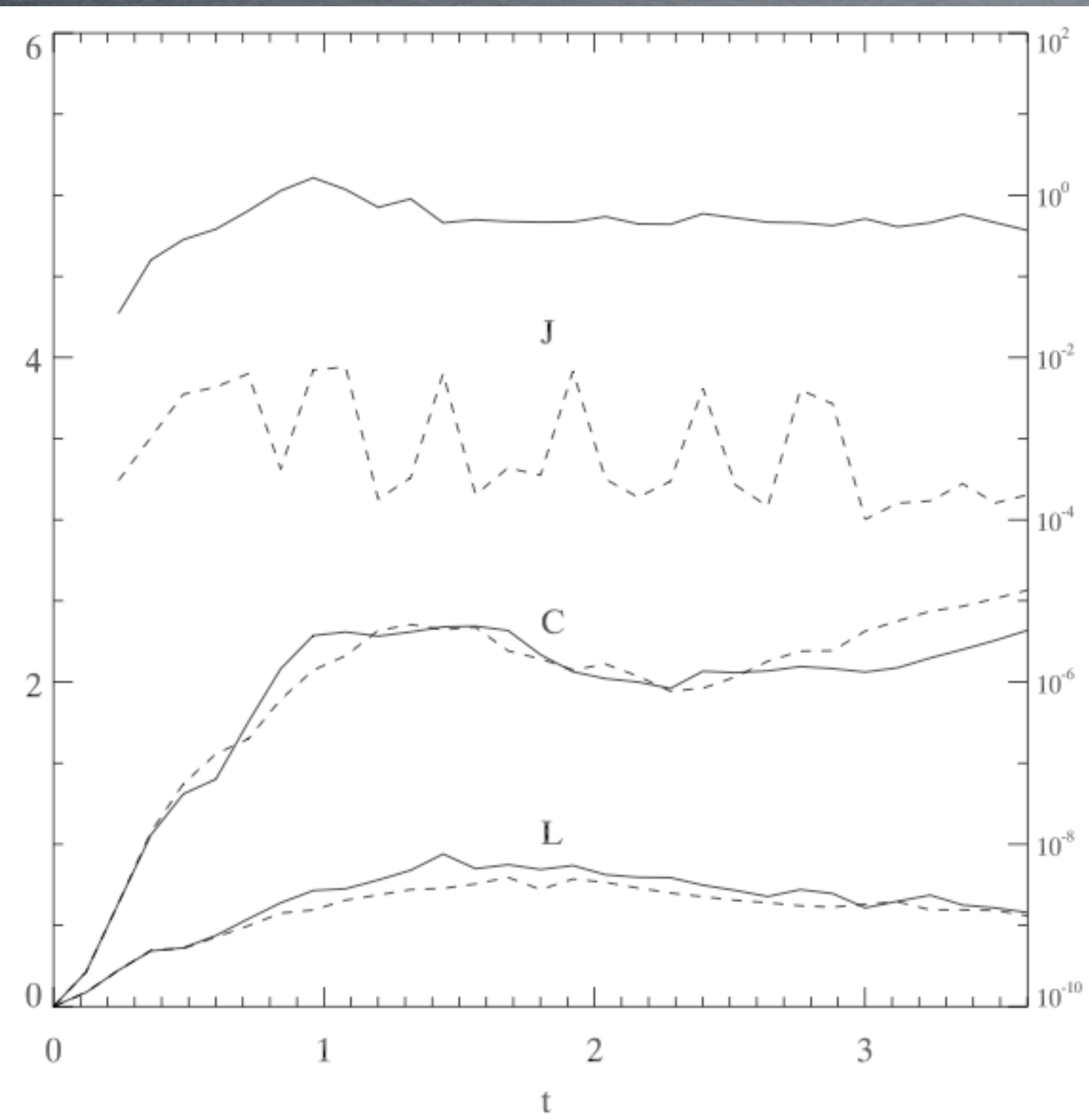
- Passive advection shows improved mass conservation/ shape preservation.

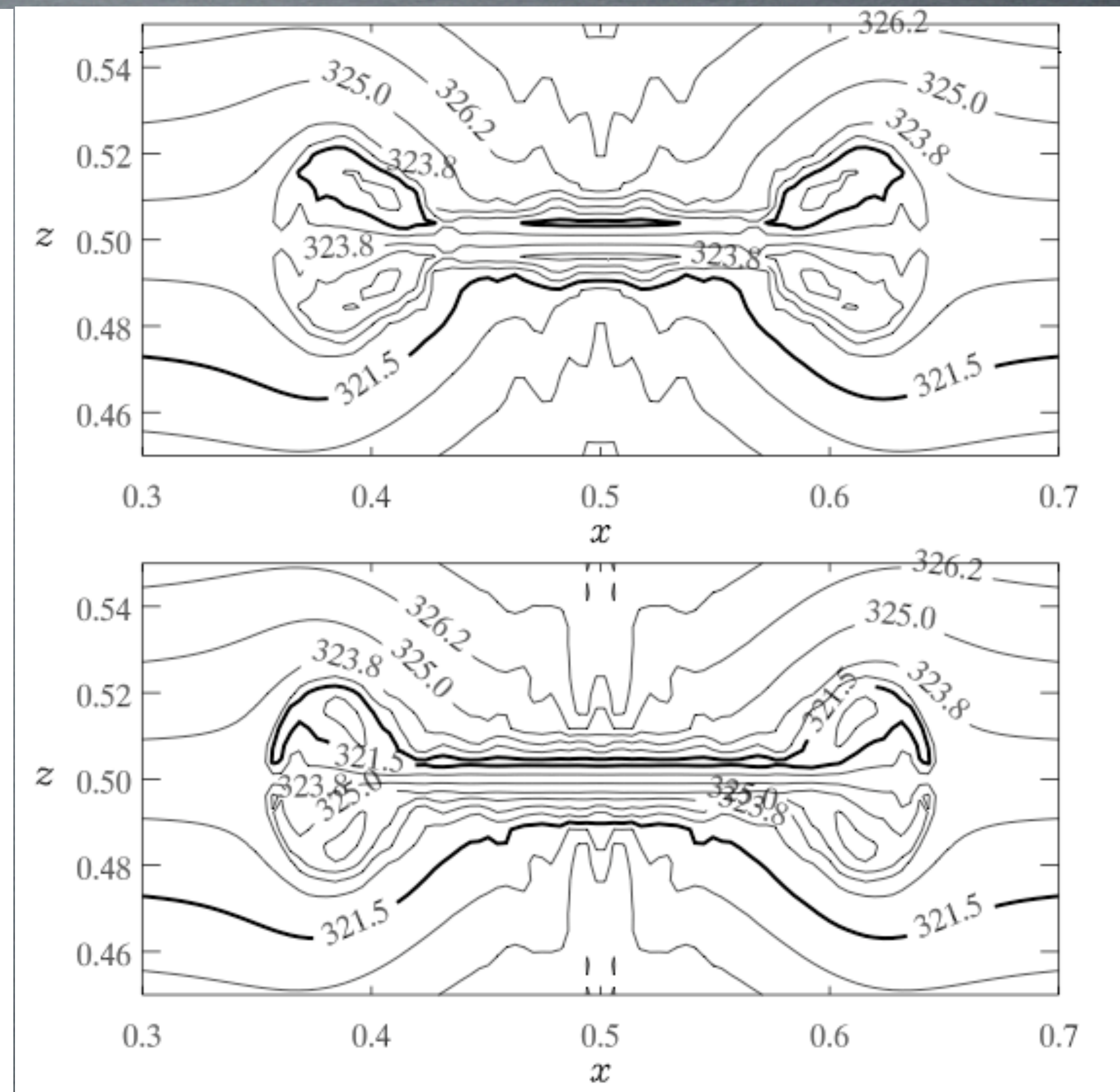
Gravitational collapse



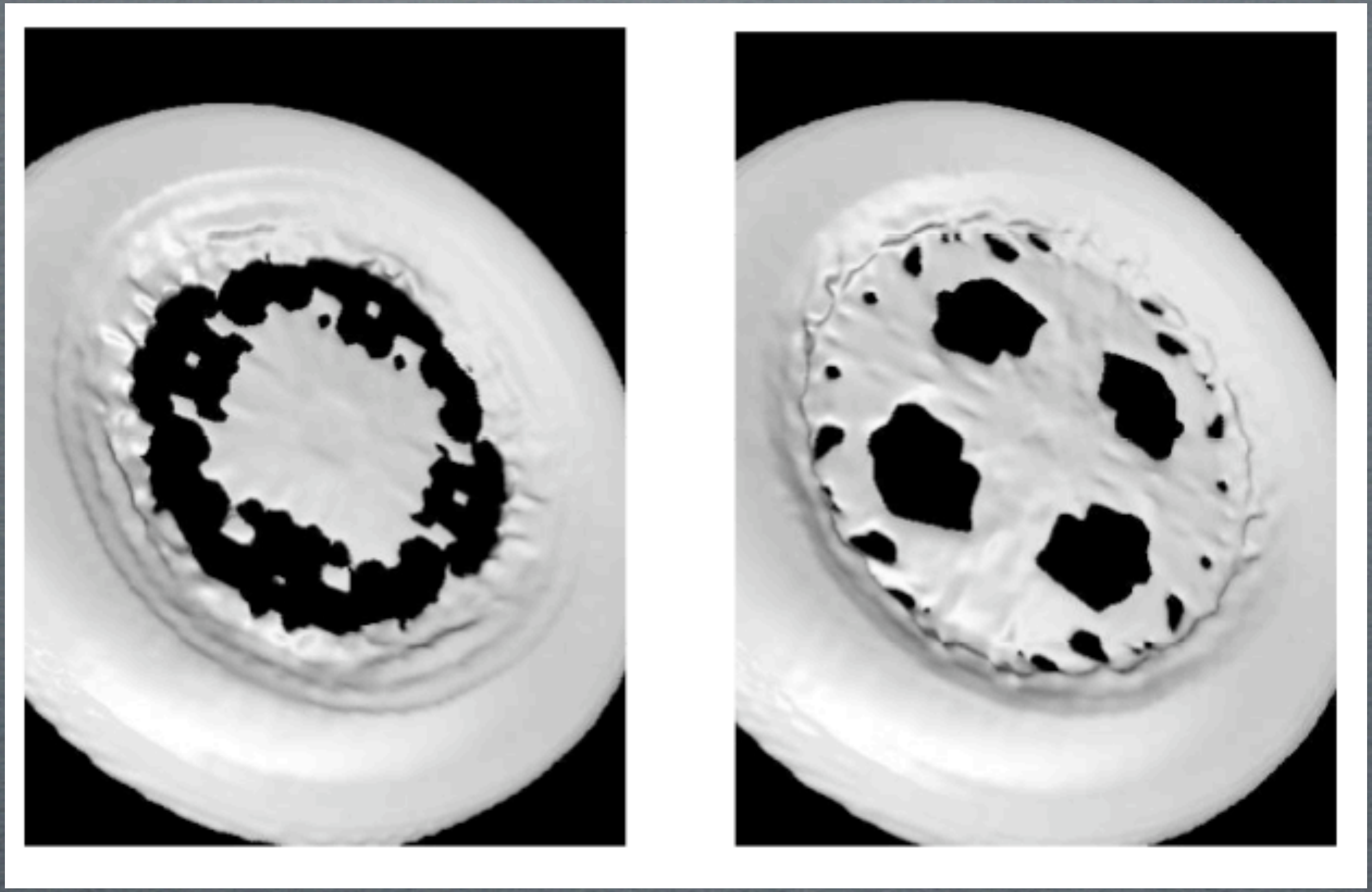
- Inviscid fluid: topology of isotherms cannot change.

Gravitational collapse

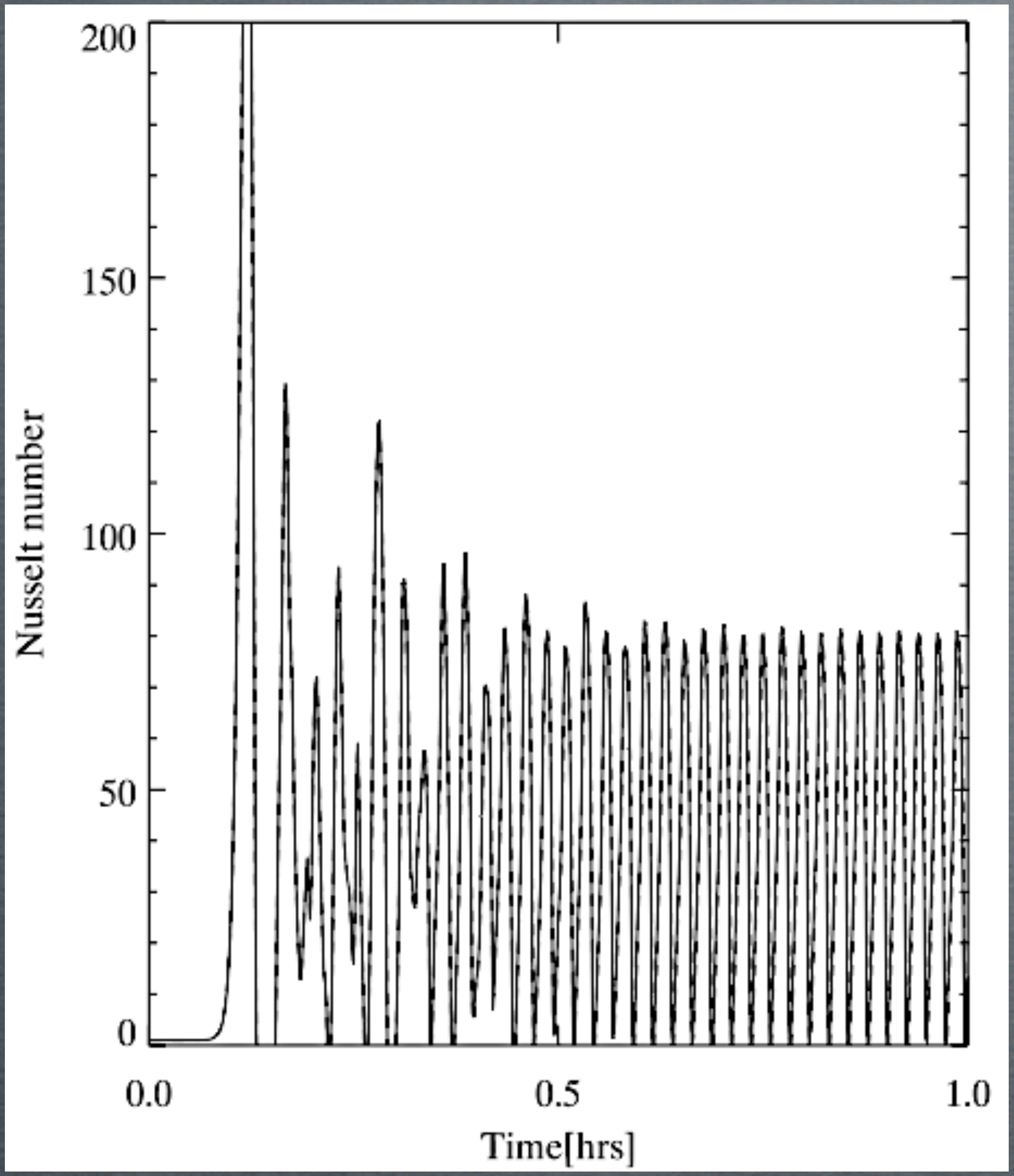


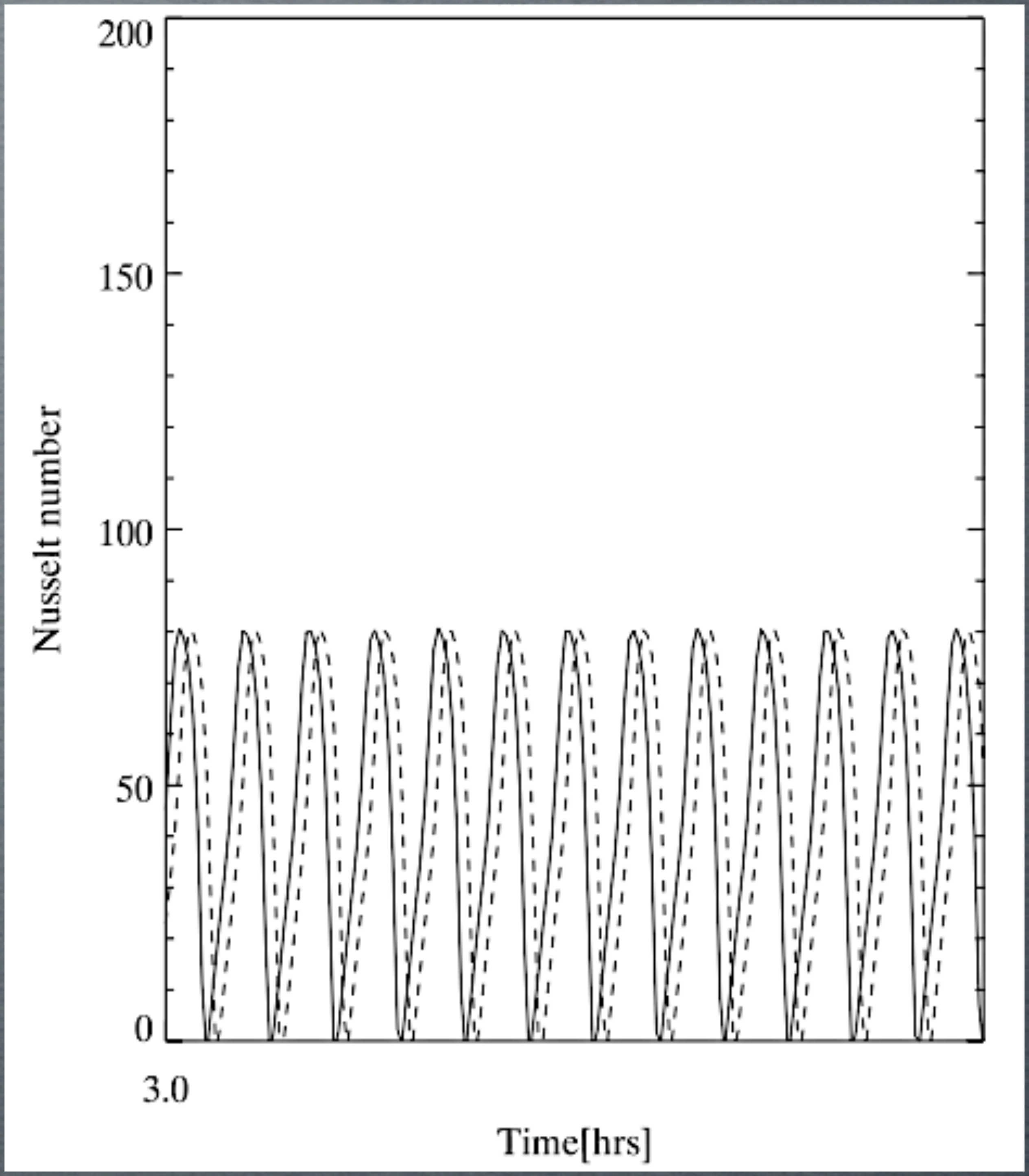


Gravitational collapse



Dealing with open boundaries- forced convection





Dealing with open boundaries- forced convection

```
illim=1
iulim=np
jllim=1
julim=mp
kllim=2
kulim=l-1

do i=illim,iulim
 do j=jllim,julim
  do k=kllim,kulim
  x00(i,j,k)=xc(i,j,k)+px(i,j,k)
  y00(i,j,k)=yc(i,j,k)+py(i,j,k)
  z00(i,j,k)=zc(i,j,k)+pz(i,j,k)
  enddo
  x00(i,j,1)=xc(i,j,1)+    px(i,j,1)
  y00(i,j,1)=yc(i,j,1)+    py(i,j,1)
  z00(i,j,1)=zc(i,j,1)+0.*pz(i,j,1)
  x00(i,j,l)=xc(i,j,l)+    px(i,j,l)
  y00(i,j,l)=yc(i,j,l)+    py(i,j,l)
  z00(i,j,l)=zc(i,j,l)+0.*pz(i,j,l)
 enddo
enddo
```

```
GCR(k)
    0.8046E-03 0.2999E-03 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.2093E-06
 line search iinit, ffcs/ffc0=,ff0=,ffc= 0.3727E+00 0.8046E-03 0.2999E-03
end of line search
GCR(k)
    0.2999E-03 0.2000E-03 0.1245E-03 0.8940E-04 0.7273E-04
    0.6395E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.2093E-06
 line search iinit, ffcs/ffc0=,ff0=,ffc= 0.2132E+00 0.2999E-03 0.6395E-04
end of line search
GCR(k)
    0.6395E-04 0.4626E-04 0.4148E-04 0.3914E-04 0.3568E-04
    0.2519E-04 0.1921E-04 0.1761E-04 0.1586E-04 0.1706E-04
    0.1353E-04 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.2093E-06
 line search iinit, ffcs/ffc0=,ff0=,ffc= 0.2116E+00 0.6395E-04 0.1353E-04
end of line search
GCR(k)
    0.1326E-04 0.1067E-04 0.9833E-05 0.1046E-04 0.1034E-04
    0.1140E-04 0.1073E-04 0.1031E-04 0.8237E-05 0.7113E-05
    0.8853E-05 0.6244E-05 0.5302E-05 0.4141E-05 0.3296E-05
    0.2089E-05 0.1405E-05 0.1012E-05 0.6479E-06 0.5411E-06
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00 0.0000E+00
    0.2093E-06
 line search iinit, ffcs/ffc0=,ff0=,ffc= 0.4000E-01 0.1353E-04 0.5412E-06
end of line search
```

•Current work: Flux expulsion in MHD.

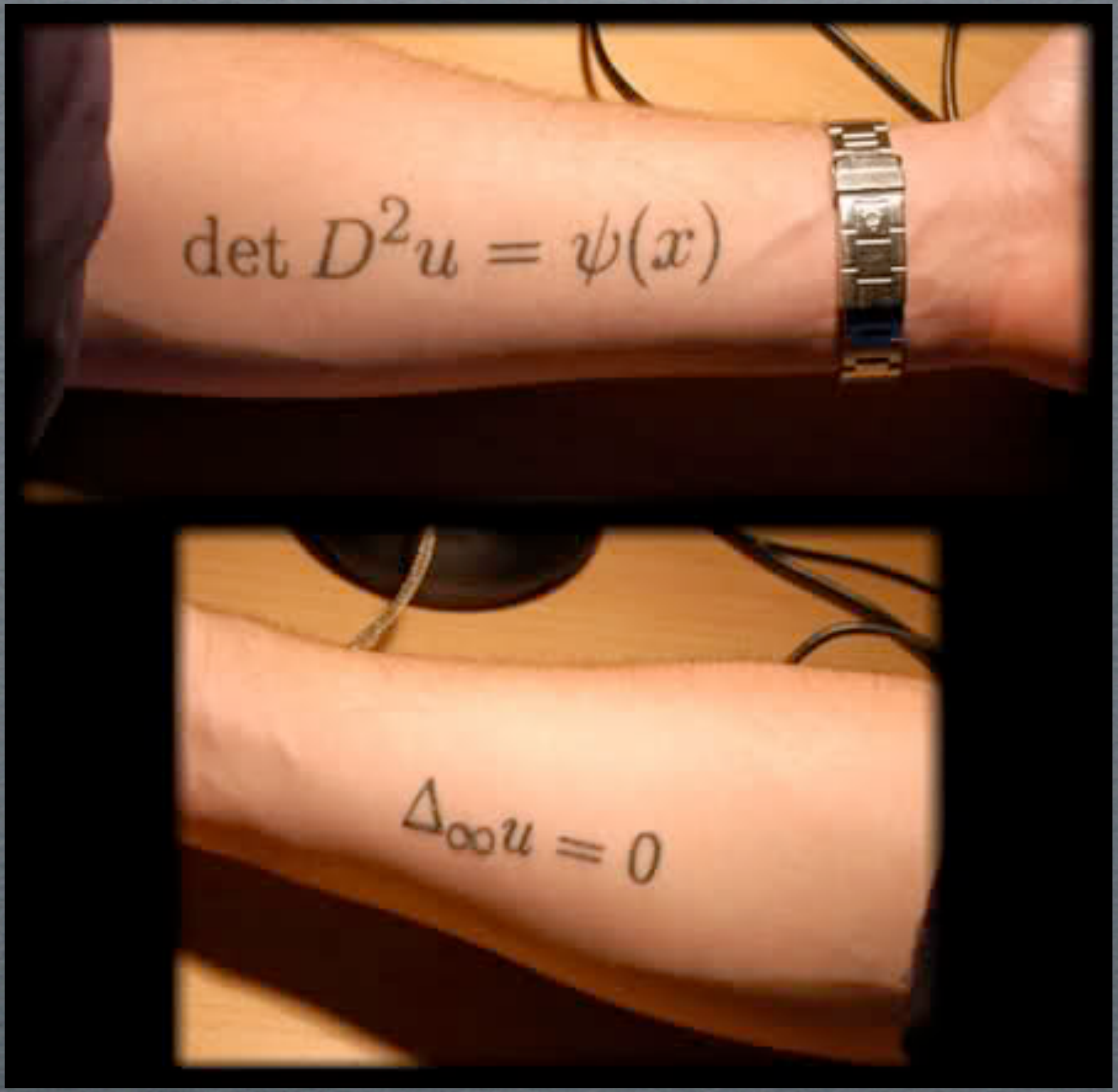
•Next: extension to anelastic and fully compressible flow.

$$\rho(\mathbf{x_i}, t) = \widehat{\mathrm{J}}\rho(\mathbf{x}_0, t_0)$$

$$\det\left\{\frac{\partial(\tilde{\mathbf{x}}_0)_C}{\partial \mathbf{x}}\right\} = \frac{\rho(\mathbf{x_i}, t)}{\rho(\mathbf{x}_0, t_0)}$$

•Density field at the foot of trajectory depends on departure point prediction and vice-versa.

•Eventually: Curvilinear coordinate



Thank you!