Numerical Models of Geophysical Fluids and Living Cells

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Outline

Section 1

Fluidos Geofísicos

Large Scale *Ocean Equations*

- The ocean: A slightly compressible fluid endowed with Coriolis and buoyancy forces
- Fundamental **hypothesis** considered (for *simplifying* physical laws):

1. Boussinesq hypothesis
2. Thin aspect ratio

Large Scale Ocean Equations

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- Fundamental **hypothesis** considered (for *simplifying* physical laws):

1. Boussinesq hypothesis ⟶

Boussinesq Hypothesis

- **Density** is a *constant* $\rho_\star$ *except in buoyancy* terms.

2. Thin aspect ratio

Large Scale *Ocean Equations*

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1. Boussinesq hypothesis
2. Thin aspect ratio →

Thin aspect ratio

- Anisotropic (flat) **domain**

$$\boxed{\varepsilon = \frac{\textit{vertical}\text{ scales}}{\textit{horizontal}\text{ scales}}}$$ is **small**

$10^{-3}, 10^{-4}$

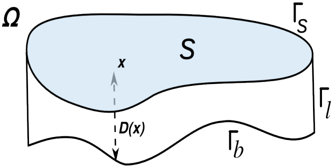
E.g. Mediterranean and North Atlantic: $\varepsilon \simeq 10^{-4}$

- Then the problem is rescaled:

$\boxed{\text{Anisotropic domain}} \to \boxed{\text{Isotropic domain}}$

The adimensional domain

- After **vertical scaling**, we obtain an **isotropic domain** $\Omega \subset \mathbb{R}^3$:



$$\varepsilon = \frac{\textit{vertical}\ \text{scales}}{\textit{horizontal}\ \text{scales}} \sim 1$$

- Cartesian coordinates and **rigid lid hypothesis** (flat surface).

  Also free surface models might be handled by our schemes.

  Non-fundamental hypothesis!

- Vertical scaling the domain $\Rightarrow$ Vertical scaling the equations...

Large-Scale Boussinesq Equations (variable density)

Anisotropic equations

Conservation of momentum and continuity

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla_{\mathbf{x}}\mathbf{u} + v\,\partial_z\mathbf{u} - \Delta_\nu \mathbf{u} + \frac{1}{\rho_\star}\nabla_{\mathbf{x}} p = \mathbf{F}_{\mathbf{u}};$$

$$\boxed{\varepsilon^2\Big(\partial_t v + \mathbf{u}\cdot\nabla_{\mathbf{x}} v + v\,\partial_z v - \Delta_\nu v\Big)} + \frac{1}{\rho_\star}\partial_z p + \frac{\rho\, g}{\rho_\star} = 0$$

$$\nabla\cdot\mathbf{u} + \partial_z v = 0$$

Convection-diffusion of *temperature* and *salinity* + state equation (density)

$$\partial_t T + (\mathbf{u}\cdot\nabla_{\mathbf{x}})T + (v\cdot\partial_z)T - \nu_T\Delta T = F_T$$

$$\partial_t S + (\mathbf{u}\cdot\nabla_{\mathbf{x}})S + (v\cdot\partial_z)S - \nu_S\Delta S = F_S$$

$$\rho = \rho_\star\big(1 - \beta_T(T - T_\star) + \beta_S(S - S_\star)\big)$$

Large-Scale Boussinesq Equations (variable density)

Variable **density** (coupling temperature and density)

Conservation of momentum and continuity

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla_{\mathbf{x}}\mathbf{u} + v\,\partial_z \mathbf{u} - \Delta_\nu \mathbf{u} + \frac{1}{\rho_\star}\nabla_{\mathbf{x}} p = \mathbf{F}_{\mathbf{u}};$$

$$\varepsilon^2\Big(\partial_t v + \mathbf{u}\cdot\nabla_{\mathbf{x}} v + v\,\partial_z v - \Delta_\nu v\Big) + \frac{1}{\rho_\star}\partial_z p + \frac{\boxed{\rho}\,g}{\rho_\star} = 0$$

$$\nabla\cdot\mathbf{u} + \partial_z v = 0$$

Convection-diffusion of *temperature* and *salinity* + state equation (density)

$$\partial_t T + (\mathbf{u}\cdot\nabla_{\mathbf{x}})T + (v\cdot\partial_z)T - \nu_T\Delta T = F_T$$

$$\partial_t S + (\mathbf{u}\cdot\nabla_{\mathbf{x}})S + (v\cdot\partial_z)S - \nu_S\Delta S = F_S$$

$$\boxed{\rho} = \rho_\star\big(1 - \beta_T(T - T_\star) + \beta_S(S - S_\star)\big)$$

Constant Density Case

Constant density hypothesis $\Rightarrow$ we focus on momentum equations:

Quasi-Hydrostatic or Anisotropic Navier-Stokes equations

$$\begin{aligned} \partial_t \mathbf{u} + \mathbf{u} \cdot \nabla_{\mathbf{x}} \mathbf{u} + v\, \partial_z \mathbf{u} - \Delta_\nu \mathbf{u} + \nabla_{\mathbf{x}} p &= \mathbf{F}_{\mathbf{u}} \\ \varepsilon^2 \left(\partial_t v + \mathbf{u} \cdot \nabla_{\mathbf{x}} v + v\, \partial_z v - \Delta_\nu v \right) + \partial_z p &= 0 \\ \nabla \cdot \mathbf{u} + \partial_z v &= 0 \end{aligned}$$

Hard problem:

- Navier-Stokes is one of the **millenium problems**
  - Transient **nonlinear** & **mixed** system of PDE equations
- New difficulties due to $\boxed{\textbf{anisotropy}}$

Steady Linear Case

Anisotropic Stokes equations

$$
\begin{aligned}
-\Delta \mathbf{u} + \nabla_{\mathbf{x}} p &= \mathbf{f},\\
-\boxed{\varepsilon}\Delta v + \partial_z p &= g,\\
\nabla_{\mathbf{x}} \cdot \mathbf{u} + \partial_z v &= 0.
\end{aligned}
$$

- When $\varepsilon \to 0$, we only expect

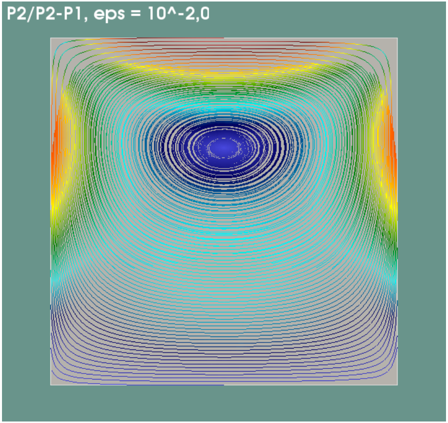
$$v \in H^1_z(\Omega) = \left\{ \overline{v} \in L^2(\Omega), \partial_z \overline{v} \in L^2(\Omega) \right\}$$

- What happens when v looses regularity?...

Not Easy Task!

Classical $\mathbb{P}_2/\mathbb{P}_1$ FE, Velocity

$\boxed{\varepsilon = 10^{-2}}$



Not Easy Task!

Classical $\mathbb{P}_2/\mathbb{P}_1$ FE, Velocity

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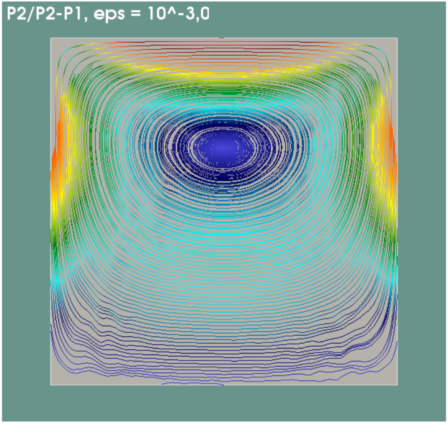
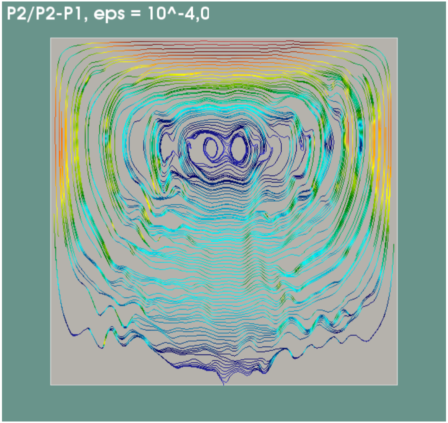
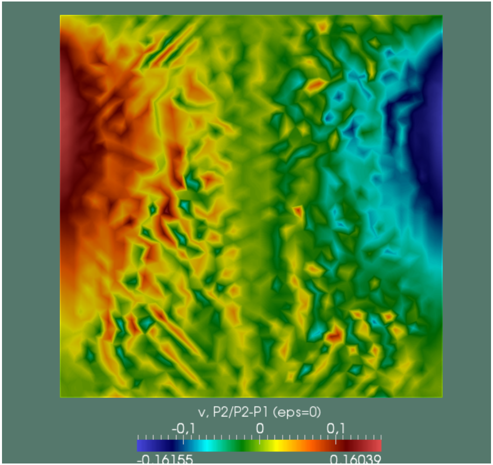


Not Easy Task!

Classical $\mathbb{P}_2/\mathbb{P}_1$ FE, Velocity

$$\boxed{\varepsilon = 10^{-4}}$$





When $\varepsilon \to 0$, coercivity for v is lost!!

A Well-Known 1-Dimensional Example

See e.g. [QSS00]

Convection-Diffusion Equation

$$-\varepsilon\, u''(x) + b\, u'(x) = 0 \quad \text{in } \Omega = (0,1) \subset \mathbb{R},$$
$$u(0) = 0, \quad u(1) = 1.$$

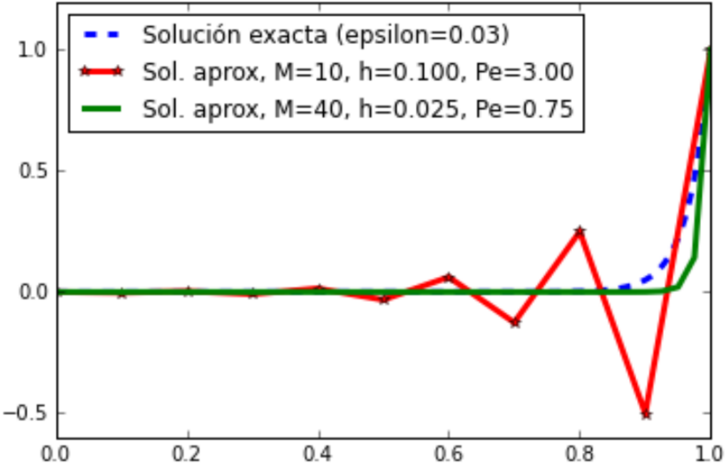
- Bilinear form: $a(u,v) = \varepsilon \int_\Omega u'v' + b \int_\Omega u'v$

  (coercivity constant vanishes if $\varepsilon \to 0$)

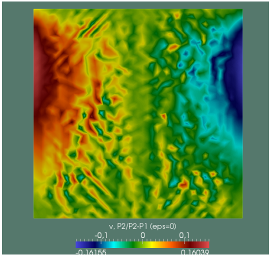
- We compute the FE solution in a partition, $\{x_i\}_{i=0}^M$ of Ω:

$$u_i = u_h(x_i) = \frac{\left(\frac{1+Pe}{1-Pe}\right)^i - 1}{\left(\frac{1+Pe}{1-Pe}\right)^M - 1}, \quad i = 1, \ldots, M-1,$$

If $Pe := \frac{bh}{2\varepsilon} > 1$ (i.e. $\varepsilon << b$), non-realistic oscillations!


Solución exacta (epsilon=0.03)
Sol. aprox, M=10, h=0.100, Pe=3.00
Sol. aprox, M=40, h=0.025, Pe=0.75
1.0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0

Ideas for Fixing Vertical Velocity Coercivity



- Different FE approximations for horizontal and vertical velocity
- Stabilize vertical velocity by additional terms
- Use Discontinous Galerkin $\mathbb{P}_k^d - \mathbb{P}_k^d$ approximations for

Velocity—Pressure!

Section 2

SIP Discontinous Galerkin

Model Problem

- Let $\Omega \subset \mathbb{R}^d, \quad \partial\Omega = \Gamma_D \cup \Gamma_N$
- We consider the simple elliptic (coercive) problem:

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = g & \text{on } \partial\Omega \end{cases}$$

- Lax-Milgram $\Rightarrow$ $\exists!$ weak solution $u \in V = H_0^1(\Omega)$ s. t:

$$\int_\Omega \nabla u \nabla \overline{u} = \int_\Omega f \overline{u} \quad \forall \overline{u} \in V$$

And moreover: $\|u\|_V \leq \dfrac{1}{\alpha}\|f\|$

-

Discontinuous FE Spaces

- *Broken* Sobolev space:

$$H^m(\mathcal{T}_h) := \left\{u \in L^2(\Omega) \mid u \in H^m(K),\ \forall K \in \mathcal{T}_h\right\},$$

Scalar product and norm:

- $(u, v)_{H^s(\mathcal{T}_h)} = \sum_{K\in\mathcal{T}_h} (u, v)_{H^s(K)}$
- $\|u\|_{H^s(\mathcal{T}_h)} = \left(\sum_{K\in\mathcal{T}_h} \|u\|^2_{H^s(\Omega)}\right)^{1/2}$

- Particular case: broken or **discontinuous polynomials**

$$V_h^d = \mathbb{P}_k^d(\mathcal{T}_h) = \left\{v \in L^2(\Omega):\ v|_K \in \mathbb{P}_k(K),\ \forall K \in \mathcal{T}_h\right\}$$

  - Discontinuity along the **edges** of triangles
  - Then $\mathbb{P}_k^d(\mathcal{T}_h) \not\subset H^1(\Omega)$!!! (non conforming approximation)...

...how to introduce variational formulation?...

SIP (Symmetric Interior Penalty) Discontinuous Galerkin

Integration by parts in each element $\rightsquigarrow$

$$
\begin{aligned}
a_h^{\mathrm{sip},\eta}(u_h, \overline{u}_h) = \int_\Omega \nabla_h u_h \cdot \nabla_h \overline{u}_h \\
- \sum_{e \in \mathcal{E}_h} \int_e \left(\{\!\{ \nabla_h u_h \}\!\} \cdot \mathbf{n}_e [\![\overline{u}_h]\!] + [\![u_h]\!] \{\!\{ \nabla_h \overline{u}_h \}\!\} \cdot \mathbf{n}_e \right) \\
+ \eta \sum_{e \in \mathcal{E}_h} \frac{1}{h_e} \int_e [\![u_h]\!] [\![\overline{u}_h]\!], \quad \forall\, u_h, \overline{u}_h \in \mathbb{P}_k^d
\end{aligned}
$$

- $\boxed{\text{Consistency} + \text{symmetry}}$
- $\boxed{\text{Coercivity (for } \eta > 0 \text{ big enough)}}$

SIP (Symmetric Interior Penalty) Discontinuous Galerkin

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$$
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a_h^{\mathrm{sip},\eta}(u_h, \overline{u}_h) = \int_\Omega \nabla_h u_h \cdot \nabla_h \overline{u}_h \\
\boxed{- \sum_{e \in \mathscr{E}_h} \int_e \Big(\{\!\{\nabla_h u_h\}\!\} \cdot \mathbf{n}_e [\![\overline{u}_h]\!] + [\![u_h]\!] \{\!\{\nabla_h \overline{u}_h\}\!\} \cdot \mathbf{n}_e \Big)} \\
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$$
\begin{aligned}
a_h^{\mathrm{sip},\eta}(u_h, \overline{u}_h) = {} & \int_\Omega \nabla_h u_h \cdot \nabla_h \overline{u}_h \\
& - \sum_{e \in \mathscr{E}_h} \int_e \left(\{\!\{\nabla_h u_h\}\!\} \cdot \mathbf{n}_e \, [\![\overline{u}_h]\!] + [\![u_h]\!] \, \{\!\{\nabla_h \overline{u}_h\}\!\} \cdot \mathbf{n}_e \right) \\
& + \boxed{\eta \sum_{e \in \mathscr{E}_h} \frac{1}{h_e} \int_e [\![u_h]\!] \, [\![\overline{u}_h]\!]}, \qquad \forall\, u_h, \overline{u}_h \in \mathbb{P}_k^d
\end{aligned}
$$

- Consistency + symmetry
- Coercivity (for $\eta > 0$ big enough)

SIP (Symmetric Interior Penalty) Bilinear Form II

Lemma (Coercivity and Continuity)

- *For $\eta \geq \eta^\star$, exists $C(\eta) > 0$ such that*

$$a_h^{\mathrm{sip},\eta}(u_h, u_h) \geq C(\eta) \|u_h\|_{\mathrm{sip}}^2, \quad \forall\, u_h \in \mathbb{P}_k^d$$

- *Exists $C_{bnd} > 0$ such that*

$$a_h^{\mathrm{sip},\eta}(u_h, \overline{u}_h) \leq C_{bnd} \|u_h\|_{\mathrm{sip}} \|\overline{u}_h\|_{\mathrm{sip}}, \quad \forall\, u_h, \overline{u}_h \in \mathbb{P}_k^d$$

$$\|u\|_{\mathrm{sip}} = \left(\|\nabla_h u\|^2 + |u|_U^2 \right)^{1/2},$$
$$|u|_U = \left(\sum_{e \in \mathscr{E}_h} \frac{1}{h_e} \int_e [\![u]\!]^2 \right)^{1/2}.$$

Proof: see e.g.[?]

Anisotropic SIP Bilinear Form

$$a_h^{\mathrm{anis}}(\mathbf{w}_h, \overline{\mathbf{w}}_h) = \sum_{i=1}^{d-1} a_h^{\mathrm{sip},\eta}(u_i, \overline{u}_i) + \varepsilon\, a_h^{\mathrm{sip},\eta}(v_h, \overline{v}_h) + (1-\varepsilon) s_h^v(v_h, \overline{v}_h)$$

where

$$s_h^v(v_h, \overline{v}_h) = \sum_{e \in \mathscr{E}_h} \frac{1}{h_e} \int_e \Big([\![v_h n_z]\!] \, [\![\overline{v}_h n_z]\!] \Big).$$

- SIP DG approximation for horizontal components of velocity
- $\varepsilon \to 0$: vanishing SIP DG for vertical velocity
  $+$ increasing vertical coercivity

Well-Posedness of SIP-DG Anisotropic Stokes

Using previous $a_h^{\text{anis}}(\mathbf{w}_h, \overline{\mathbf{w}}_h)$ we can define an adequate velocity/pressure mixed bilinear form $c_h^{\text{anis}}(\cdot,\cdot)$ verifying:

Theorem (Generalized coercivity)

Assume that that $\eta > \eta_*$. Then, there exists $\gamma > 0$ independent of h such that, for all $(\mathbf{w}_h, p_h) \in \mathbf{X}_h = \mathbf{W}_h \times P_{h,0}$, one has

$$\gamma \, \|(\mathbf{w}_h, p_h)\|_{\varepsilon,\mathbf{X}_h} \leq \sup_{(\overline{\mathbf{w}}_h,\overline{p}_h)\in \mathbf{X}_h\setminus\{0\}} \frac{c_h^{\text{anis}}((\mathbf{w}_h, p_h), (\overline{\mathbf{w}}_h, \overline{p}_h))}{\|(\overline{\mathbf{w}}_h, \overline{p}_h)\|_{\varepsilon,\mathbf{X}_h}}. \tag{1}$$

According to Banach-Necas-Babuška Theorem we have:

Corollary

Well-Posedness of SIP-DG-Stokes

Section 3

Numerical Tests

Cavity tests for Anisotropic Equations

Aim: test qualitative behavior of DG solution when $\varepsilon \to 0$

- FreeFem++
- $\Omega = (0,1)^2$, mesh: $h \simeq 1/30$
- Dirichlet boundary conditions:
  - Surface boundary: Γ_s: $u_h = x(1-x)$ and $v_h = 0$
  - Bottom: (Γ_b): $u_h = 0$ and $v_h = 0$
  - Lateral walls: (Γ_l): $u_h = 0$
- Neumann boundary conditions on lateral walls Γ_l: $\varepsilon \nabla v_h \cdot \mathbf{n} = 0$
- SIP DG, $\mathbb{P}_1^d$, interior penalty: $\eta = 5$.
- As usual in DG methods, Dirichlet boundary conditions are **imposed weakly**
  - Specifically, for each jump and mean boundary term appearing in DG bilinear forms, we add a corresponding term to the RHS containing the boundary value

Test 1. Anisotropic equations, $\varepsilon = 1$ *(Stokes case)*

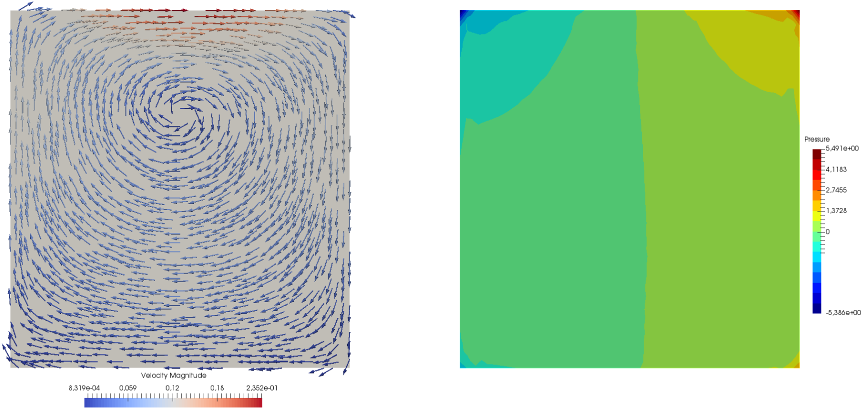

Figure 1. Cavity test, $\varepsilon = 1$.

Test 2: Anisotropic equations, $\varepsilon = 10^{-8}$ and $\varepsilon = 0$ (Hydrostatic case)

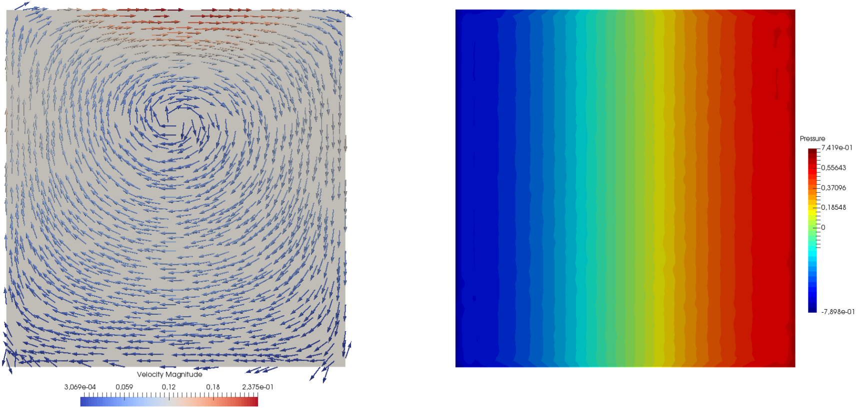

Figure 2. Cavity test, $\varepsilon = 10^{-8}$ and $\varepsilon = 0$.

Test 3. Necessity of Anisotropic Term

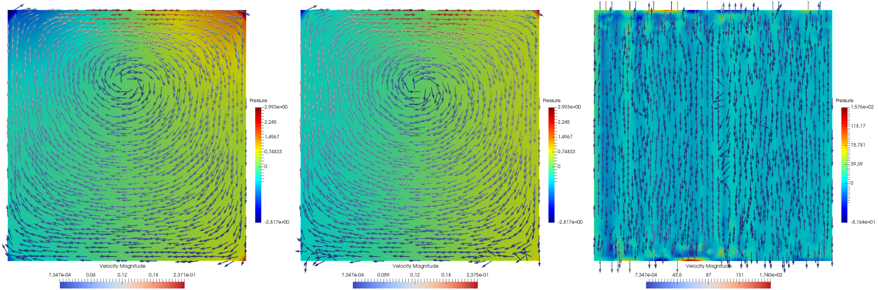

Figure 3. Anisotropic DG scheme, without the term $(1-\varepsilon)s_h^v(v_h, \overline{v}_h)$ for $\varepsilon = 1$, $\varepsilon = 10^{-2}$ and $\varepsilon = 10^{-4}$, respectively.

Section 4

Living Cell Equations

Chemotaxis

- Movement of biological cells in response to chemical signals

  → Video: neutrophile chemotaxis

- General formulation (Keller–Segel 1970') [BBTW15]

  Find u, v (density of cells and chemical-signal) such that:

$$\begin{cases} u_t = \nabla \cdot \Big(D_u(u,v)\nabla u - \chi(u,v) u \nabla v \Big) + H(u,v), \\ v_t = D_v(u,v)\Delta v + K(u,v) \end{cases}$$

- Many variants[1] depending on (likely nonlinear) terms...
  - Source terms: $H(u,v)$, $K(u,v)$
  - Diffusion of cells and chemoattractant: $D_u(u,v)$, $D_v(u,v)$

[1] See e.g. [Ho03] for a review

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The Classical Keller-Segel System

We focus on the *classical system* in $\Omega \times (0, T) \subset \mathbb{R}^{n+1}$:

$$\begin{cases} u_t = \alpha_0 \Delta u - \alpha_1 \nabla \cdot (u \nabla v), & x \in \Omega,\ t > 0, \\ v_t = \alpha_2 \Delta v - \alpha_3 v + \alpha_4 u, & x \in \Omega,\ t > 0. \end{cases}$$

- Parameters $\alpha_i > 0$. In particular $\alpha_1 > 0 \Rightarrow$ chemoattractant model
- Nolinear chemotaxis term! Hyperbolic effects expected if $\alpha_1 \gg$
- Boundary conditions

$$\frac{\partial u}{\partial \nu} = \frac{\partial v}{\partial \nu} = 0, \quad x \in \partial\Omega,\ t > 0.$$

- Initial conditions (important rule in long-time behaviour):

$$u(x,0) = u_0(x), \quad v(x,0) = v_0(x), \qquad x \in \Omega.$$

Local Existence, Positivity and Blow-up

A general result[2]:

- If $u_0 \in C^0(\overline{\Omega})$, $v_0 \in W^{1,q}(\Omega)$ non-negative ($q > n =$ space dim.)
- Then $\begin{cases} \exists T_{\text{max}} \in (0, +\infty] \text{ and} \\ \exists! u, v \in C^0(\overline{\Omega} \times (0, T_{\text{max}})) \end{cases}$ such that[3]
  - (u, v) solves classical Keller-Segel equations in $\Omega \times (0, T_{\text{max}})$
  - $u, v \geq 0$ (positivity of solution)
  - If $T_{\text{max}} < +\infty \Rightarrow \|u\|_{L^\infty(\Omega)} + \|v\|_{W^{1,q}(\Omega)} \to \infty$ as $t \nearrow T_{\text{max}}$
- We say that u blows up in T_{max} if $\|u\|_{L^\infty(\Omega)} \to \infty$ as $t \nearrow T_{\text{max}}$.

[2] This result is also valid for more general Keller-Segel equations see e.g. [BBTW15], Lemma 3.1

[3] In fact, also $u, v \in C^{2,1}(\overline{\Omega} \times [0, T_{\text{max}}))$ $v \in L^\infty_{\text{loc}}([0, T_{\text{max}}); W^{1,q}(\Omega))$

Other Properties

- Mass conservation: If u is a regular enough solution in $\Omega \times (0, T)$,

$$\int_\Omega u(\cdot, t) = \int_\Omega u_0 \quad \forall t \in (0, T).$$

- Energy dissipation:

$$\frac{d}{dt}\mathscr{E}\big(u(\cdot, t), v(\cdot, t)\big) = -\mathscr{D}\big(u(\cdot, t), v(\cdot, t)\big) \quad \forall t \in (0, T),$$

  with

$$\mathscr{E}(u, v) = \frac{1}{2}\int_\Omega |\nabla v|^2 + \int_\Omega v^2 - \int_\Omega uv + \int_\Omega u \ln u,$$
$$\mathscr{D}(u, v) = \int_\Omega v_t^2 + \int_\Omega \left| \frac{\nabla u}{\sqrt{u}} - \sqrt{u}\nabla v \right|^2.$$

☞ *Crucial role in theoretical results (global existence, blow-up...)*

Theorem (Global Existence and Boundedness)

- Assume $u_0 \in C^0(\overline{\Omega})$, $\quad v_0 \in \bigcup_{q>n} W^{1,q}(\Omega)$,
- Let (u, v) maximal solution of classical K-S.

Then

- If $n = 1$ or $n = 2$ $\left(\text{with } \int_\Omega u_0 < 4\pi \text{ for } n = 2\right)$[4]

  $\Rightarrow$ (u, v) *exists globally* in time and is bounded, i.e.

$$\|u(\cdot, t)\|_{L^\infty(\Omega)} + \|v(\cdot, t)\|_{L^\infty(\Omega)} \le C \quad \forall t > 0.$$

- If $n \ge 3$: $\exists \varepsilon, \lambda > 0$ such that

$$\text{if} \quad \|u_0\|_{L^{n/2}(\Omega)} < \varepsilon, \quad \|u_0\|_{W^{1,n}(\Omega)} < \varepsilon,$$

  $\Rightarrow$ (u, v) *exists globally* in time and satisfies

$$\|u(\cdot, t) - \overline{u_0}\|_{L^\infty(\Omega)} + \|v(\cdot, t) - \overline{v_0}\|_{L^\infty(\Omega)} \le Ce^{-\lambda t} \quad \forall t > 0.$$

[4] It is enough $\int_\Omega u_0 < 8\pi$ if Ω is a disc and (u_0, v_0) radially symmetric

Section 5

Time Schemes

Time Discretization

Let

- $0 = t_0 < t_1 < \cdots < t_N = T$
- $k = t_{m+1} - t_m, \quad u^m \approx u(t_m), \quad \forall m = 0, ..., N$

Euler Time Scheme Family

$$(1/k)u^{m+1} - \Delta u^{m+1} + \nabla \cdot (u^{m+s_1} \nabla v^{m+s_2}) = (1/k)u^m$$

$$(1/k)v^{m+1} - \Delta v^{m+1} + v^{m+s_3} - u^{m+s_4} = (1/k)v^m$$

where $S = (s_1, s_2, s_3, s_4) \in \{0, 1\}^4$.

- All of them are implicit; the scheme $S = (1, 1, 1, 1)$ is fully implicit
- We are interested discrete energy laws for linear and uncoupled schemes

Proposition (Discrete Energy Laws)

If $\big\{(u^m, v^m)\big\}_{m=0}^N$ sufficiently regular solution of scheme $S = (s_1, s_2, s_3, s_4)$:

$$\delta_t \mathscr{E}_S^{m+1} \le -\mathscr{D}_S^{m+1} - \mathscr{N}_S^{m+1} + \mathscr{M}_S^{m+1}, \quad \forall m = 0, \dots, N-1,$$

where

$$\mathscr{E}_S^{m+1} = \mathscr{E}(u^{m+1}, v^{m+1}),$$

$$\mathscr{D}_S^{m+1} = \int_\Omega \left(\delta_t v^{m+1}\right)^2 + \int_\Omega \left| \frac{\nabla u^{m+1}}{\sqrt{u^{m+1}}} - \sqrt{u^{m+1}} \nabla v^{m+1} \right|^2,$$

$$\mathscr{N}_S^{m+1} = \frac{k}{2} \int_\Omega \left(\partial_t \nabla v^{m+1}\right)^2 + N_{1,S} + N_{2,S} + N_{3,S} + N_{4,S},$$

$$\mathscr{M}_S^{m+1} = M_{1,S} + M_{2,S} + M_{3,S} + M_{4,S}.$$

Here:

- $\delta_t(w^m) = (w^{m+1} - w^m)/k$,
- $N_{i,S}, M_{i,S} \ge 0$ (numerical dissipation and sources), $N_{i,S}, M_{i,S} \to 0$ as $k \to 0$.

Proof

Similar to continuous Energy Law, using following properties:

- $\delta_t(w^{m+1})w^{m+1} = \frac{1}{2}\delta_t(w^{m+1})^2 + \frac{k}{2}(\delta_t w^{m+1})^2 \quad \forall m \geq 0,$
- $\delta_t(u^{m+1} \cdot v^{m+1}) = u^m \partial_t v^{m+1} + v^{m+1} \partial_t u^{m+1} \quad \forall m \geq 0,$
- $b \left(\log a - \log b\right) \leq a - b \quad \forall a, b > 0,$
- $\int_\Omega \delta_t u^{m+1} = 0 \quad \forall m \geq 0$ (discrete conservation of mass).

$\square$

Optimal (?) Time Scheme: $S = (1,1,1,0)$

$$(1/k)u^{m+1} - \Delta u^{m+1} + \nabla \cdot (u^{m+1}\nabla v^{m+1}) = (1/k)u^m,$$

$$(1/k)v^{m+1} - \Delta v^{m+1} + v^{m+1} - u^m = (1/k)v^m.$$

- Uncoupled (first compute v^{m+1}, then u^{m+1})
- $N_{i,S} = 0,\ i = 1,\dots,4 \Rightarrow \mathcal{N}_S^{m+1} = \frac{k}{2}\int_\Omega \left(\partial_t \nabla v^{m+1}\right)^2$ minimizes dissipation.
- $M_{i,S} = 0,\ i = 1,\dots,4 \Rightarrow \mathcal{M}_S^{m+1} = 0$ minimizes numerical sources.

Energy law:

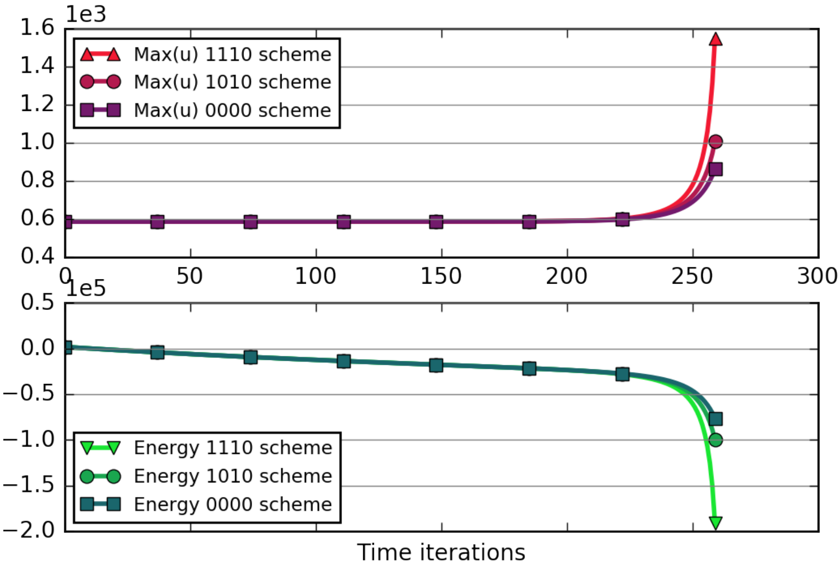
$$\delta_t \mathcal{E}_S^{m+1} \le -\mathcal{D}_S^{m+1} - \mathcal{N}_S^{m+1} \le 0 \ \Rightarrow\ \mathcal{E}_S^{m+1} \searrow 0.$$

Conjectures:

$$\delta_t \mathcal{E}_S^{m+1} = \min_{S' \in \{0,1\}^4} \delta_t \mathcal{E}_{S'}^{m+1} \ ??? \qquad \mathcal{E}_S^{m+1} = \min_{S' \in \{0,1\}^4} \mathcal{E}_{S'}^{m+1} \ ???$$

$$\|u_S^m\|_{L^\infty(\Omega)} \le \|u_{S'}^m\|_{L^\infty(\Omega)} \quad \forall S' \in \{0,1\}^4 \ ???$$

Please, Some Simulations!



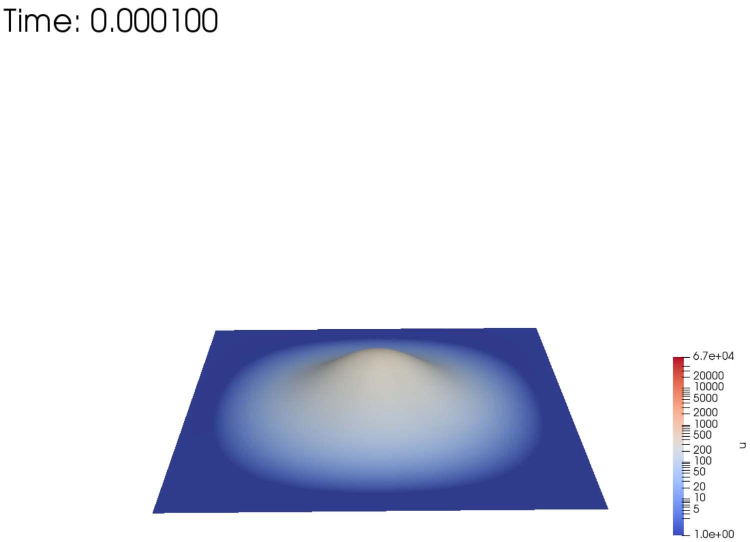
Section 6

Space Discretization

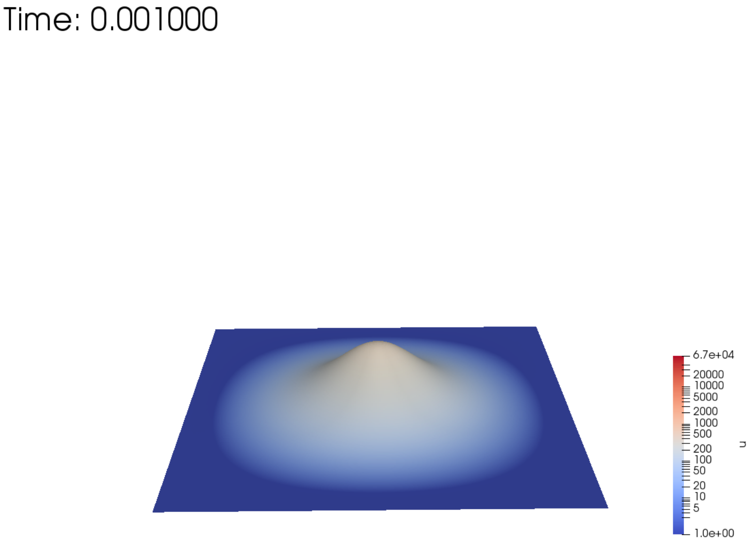
FEM Space Discretization

- For any Euler scheme $S \in \{0,1\}^4$,
  we approximate (u^m, v^m) at each time t_m by means of **FEM**
- All right (apparently)...
  e.g. let us reproduce the following **numerical test** [FMV15]:
  - $\Omega = [-2,2]^2 \subset \mathbb{R}^2$ $(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) = (1, 0.2, 1, 0.1, 1)$
  - $u_0 = 1.15 e^{-(x^2+y^2)}(4-x^2)^2(4-y^2)^2$ ($\int_\Omega u_0 > \pi/4$, blow-up!)
    $v_0 = 0.55 e^{-(x^2+y^2)}(4-x^2)^2(4-y^2)^2$
  - Time discretization: Euler scheme $S = (0,0,0,0)$
  - Discretization: P1-Lagrange 200×200 mesh ($h \sim 10^{-2}$), $k = 10^{-4}$

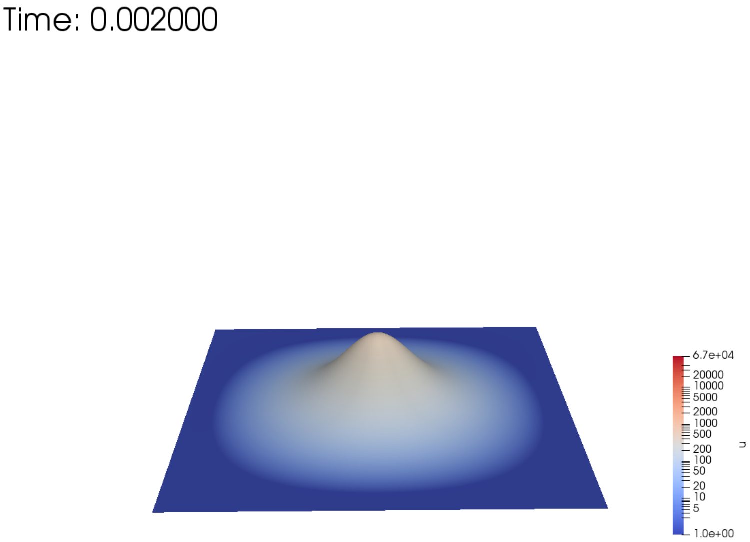
Blow-up Test (plotting u)



Blow-up Test (plotting u)



Blow-up Test (plotting u)



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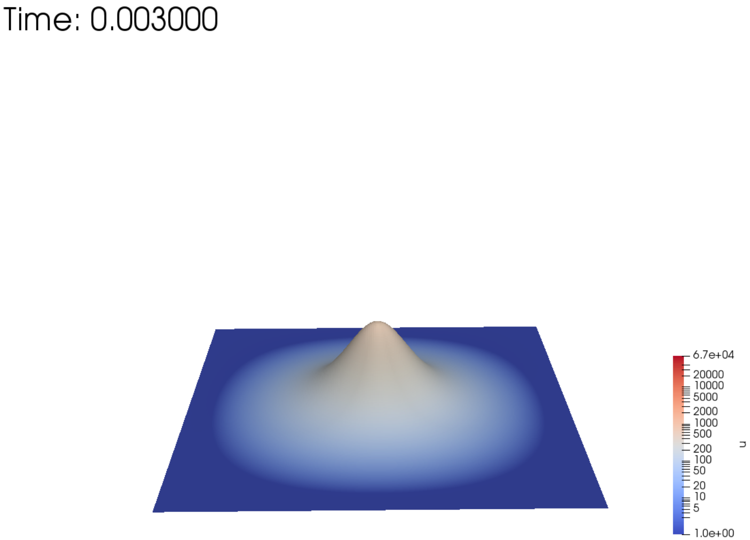

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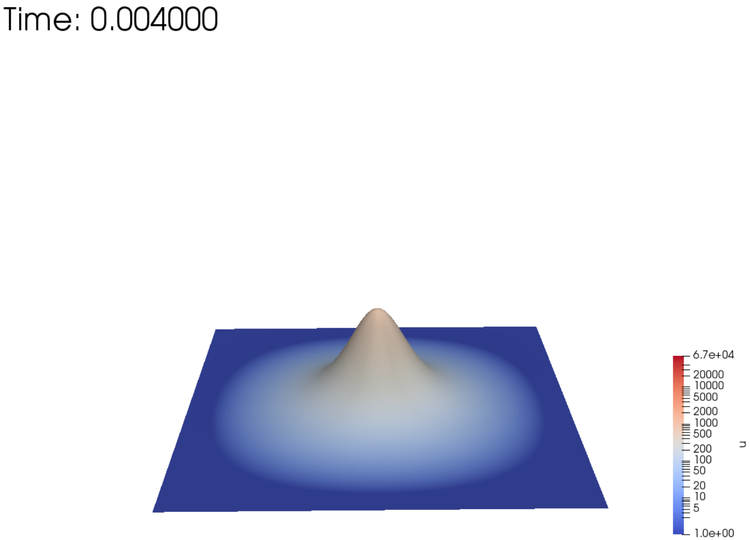

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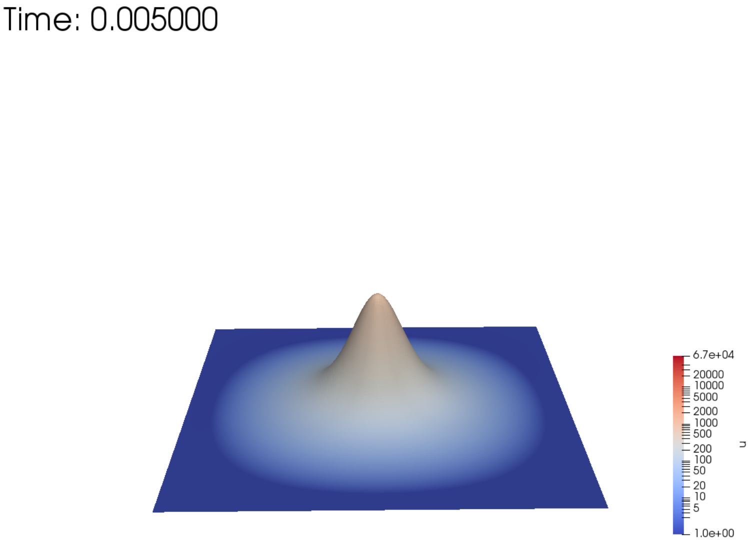
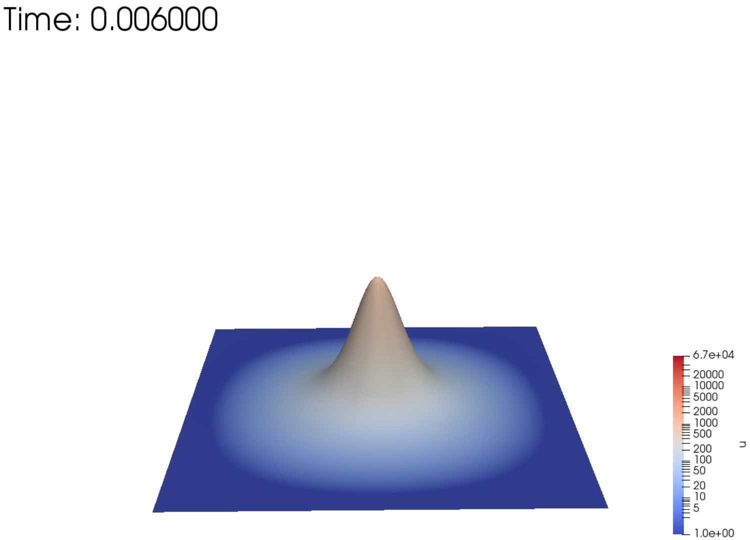
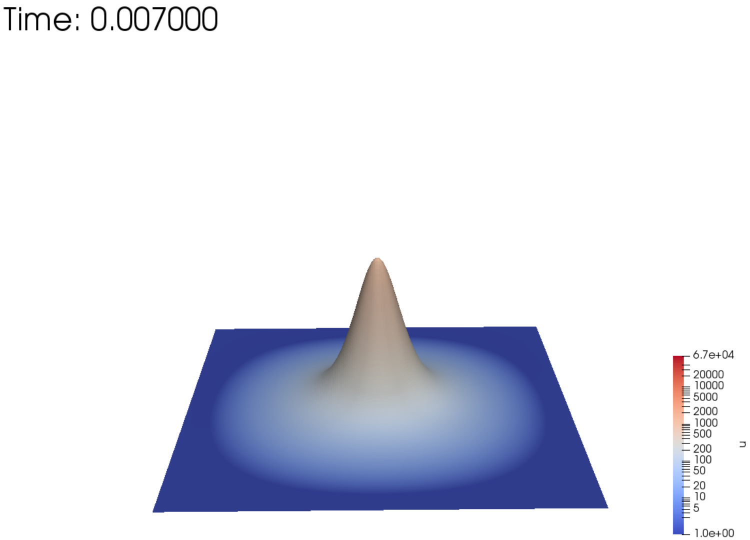


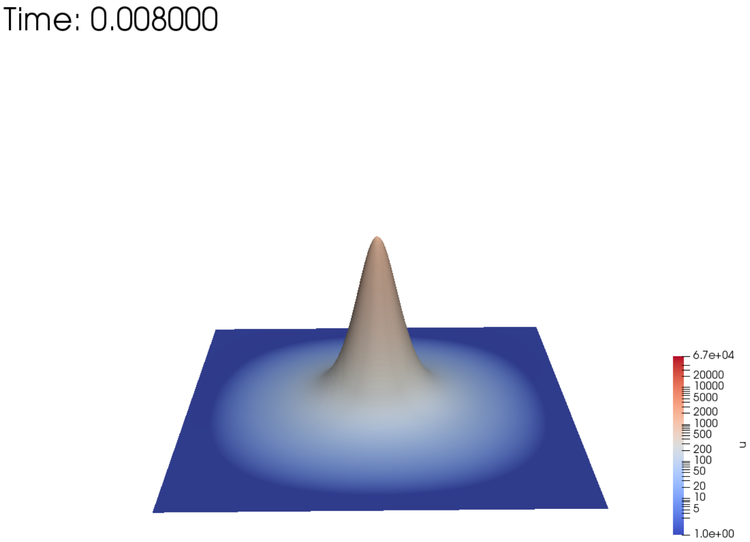
Blow-up Test (plotting u)



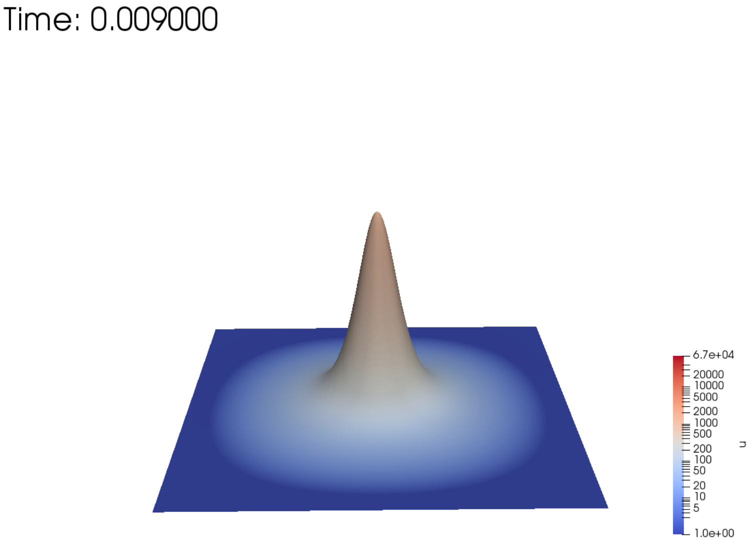
Blow-up Test (plotting u)



Blow-up Test (plotting u)

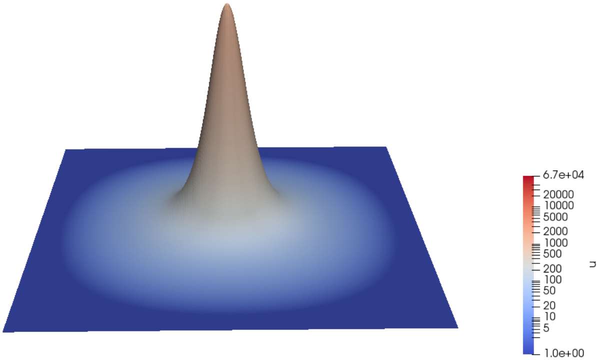


Blow-up Test (plotting u)

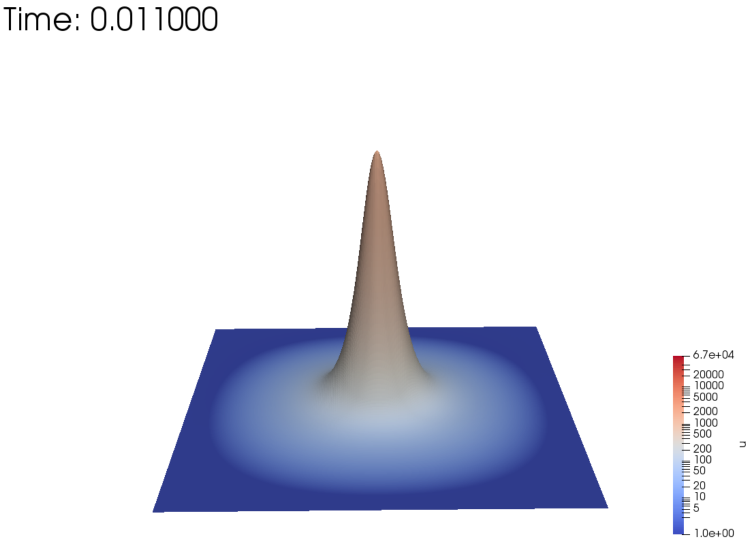


Blow-up Test (plotting u)

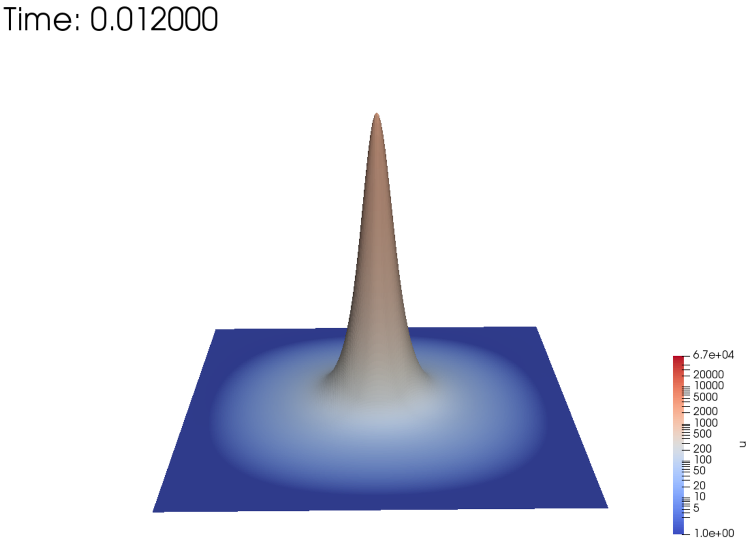
Time: 0.010000



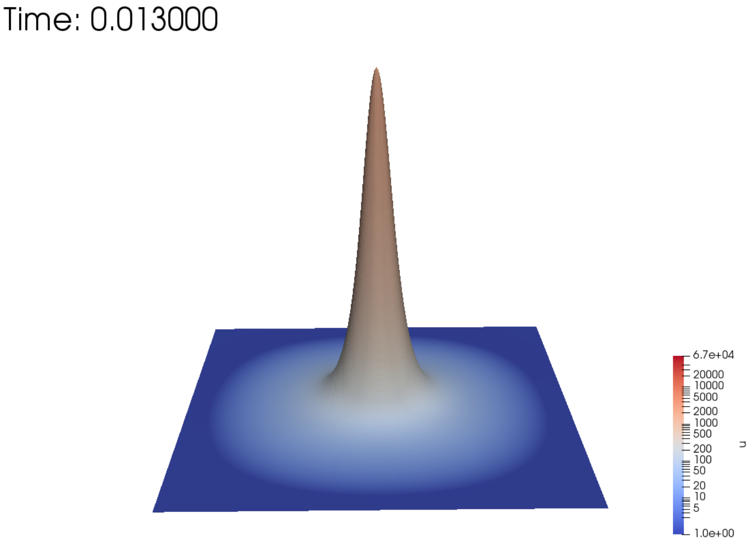
Blow-up Test (plotting u)



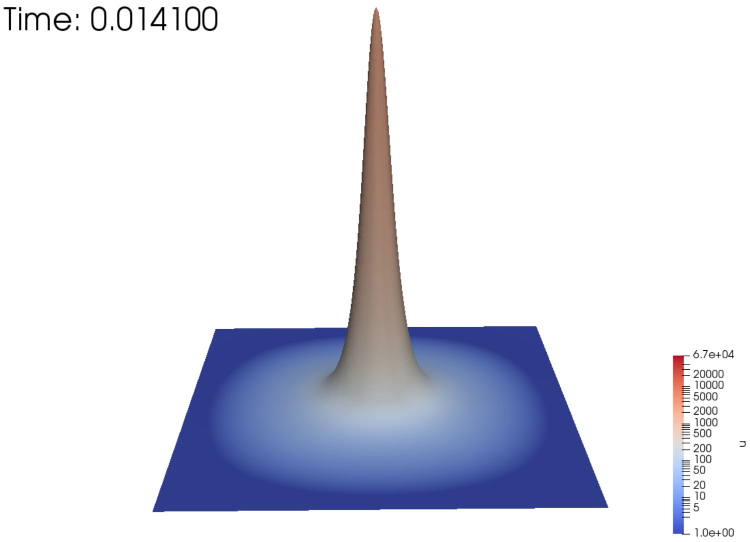
Blow-up Test (plotting u)



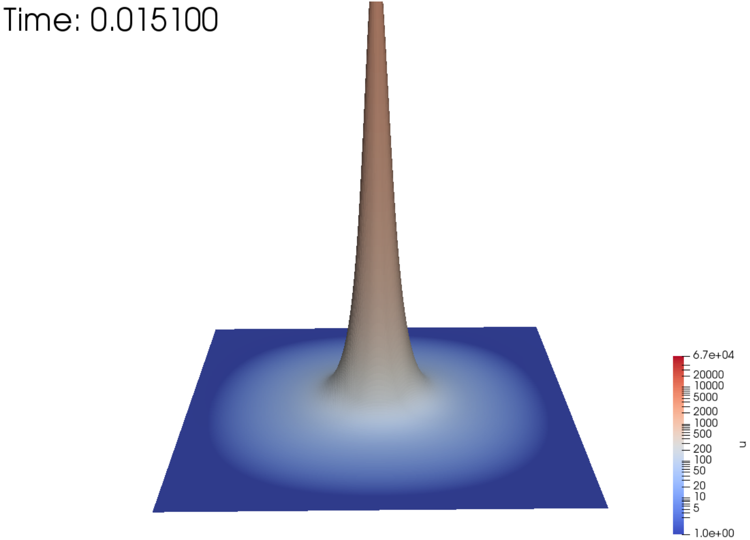
Blow-up Test (plotting u)



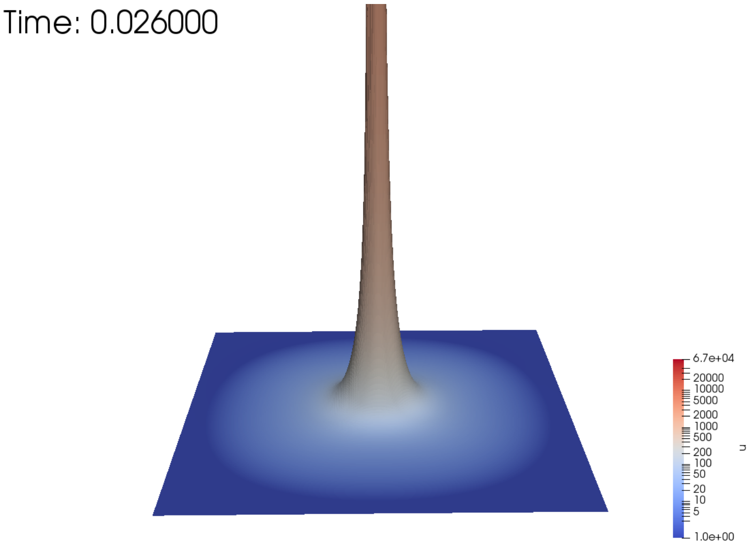
Blow-up Test (plotting u)



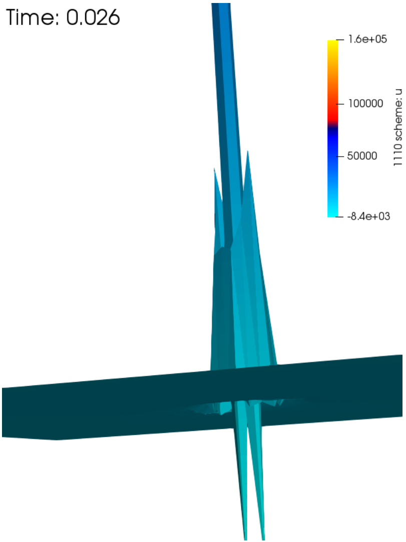
Blow-up Test (plotting u)



Blow-up Test (plotting u)

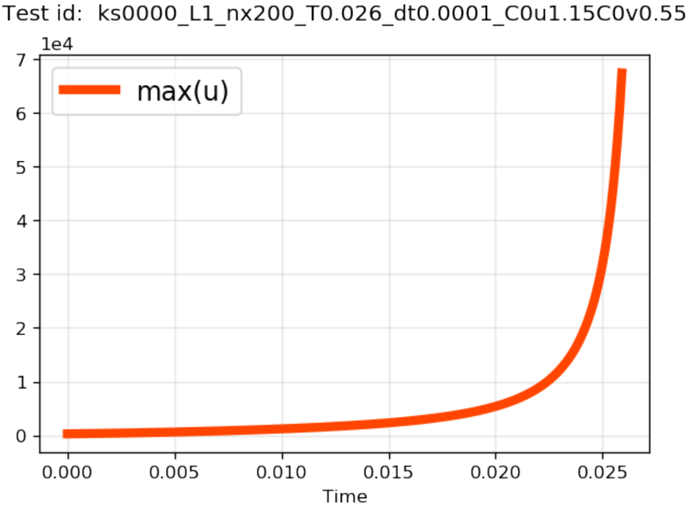


But it's not all so nice...

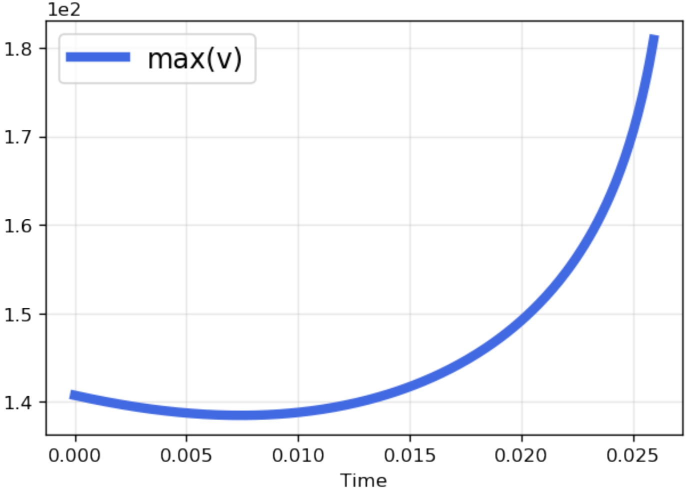


Spurious Oscillations Near Blow-up Time!

Maximum Density of Cells Over Time

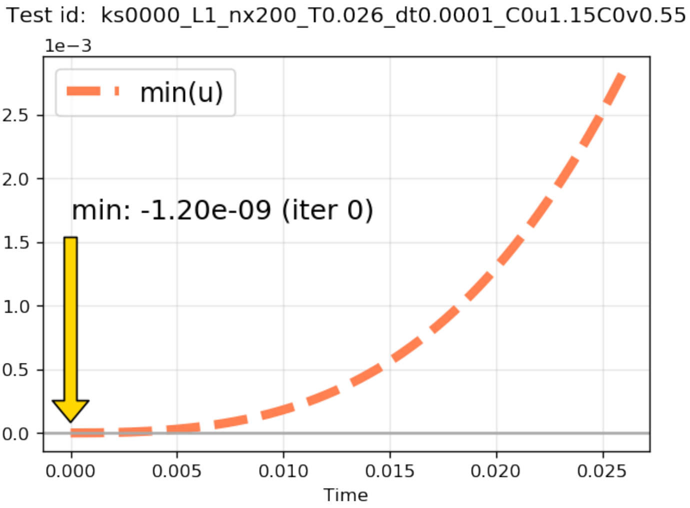


Maximum Chemical Agent Over Time



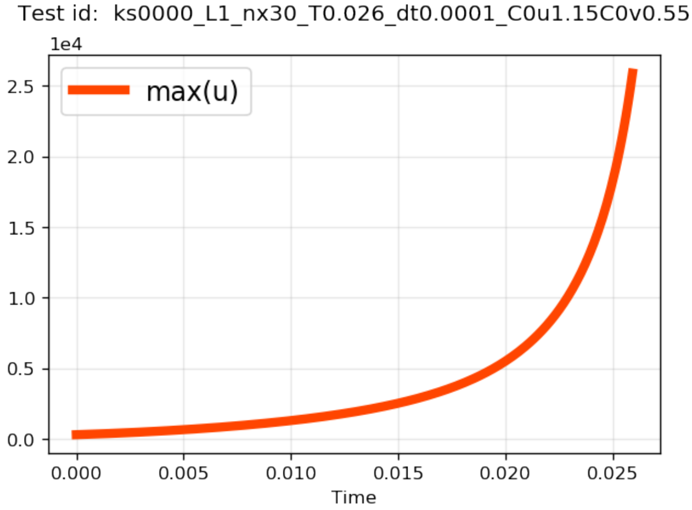
***Positivity* of u is broken due to FE approximation!**

Minimum Cells Over Time

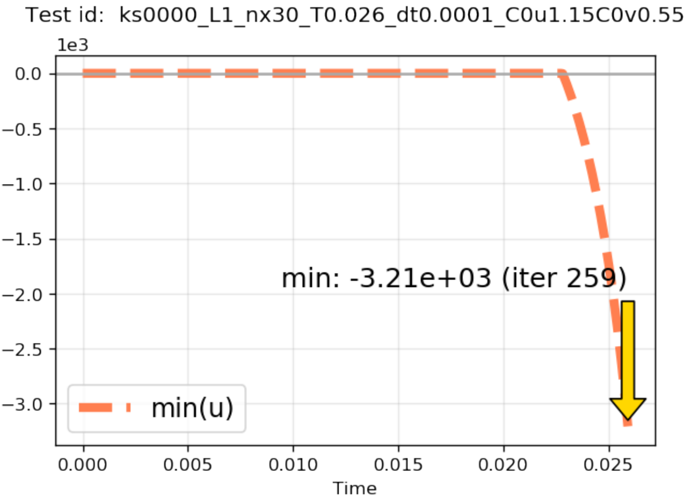


***Positivity* of u is broken due to FE approximation!**

Minimum Cells in a Coarser Grid (nx=30)

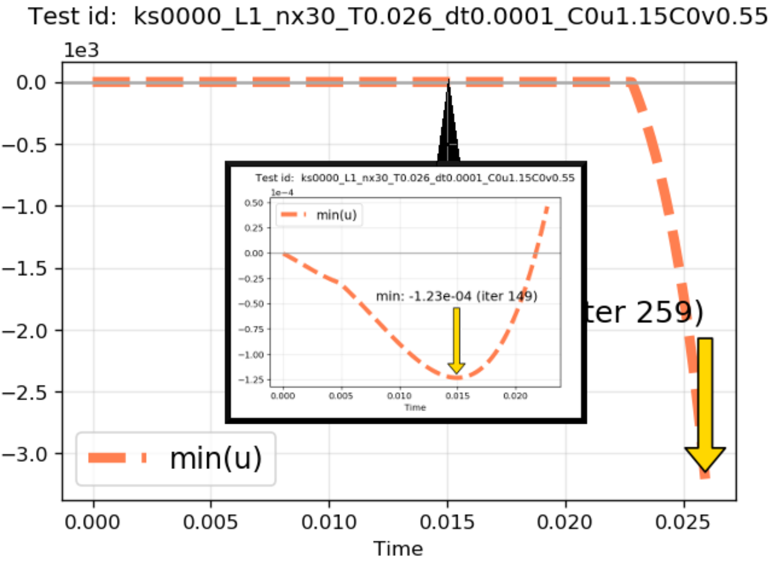


Minimum Cells in a Coarser Grid (nx=30)



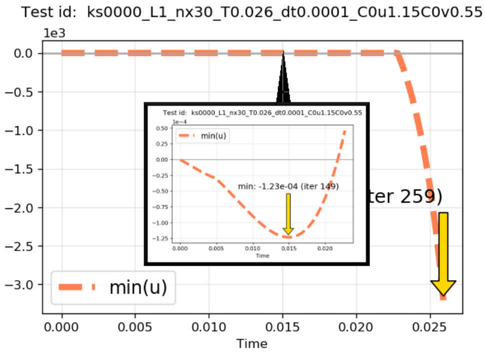
Positivity of u is broken near blow-up time

... also positivity lost at initial time!



Other Euler Schemes do Not Improve Positivity

- E.g. similar (slightly better) results are obtained for $S = (1,1,1,0)$



- Let us check other **FE space approximations**...

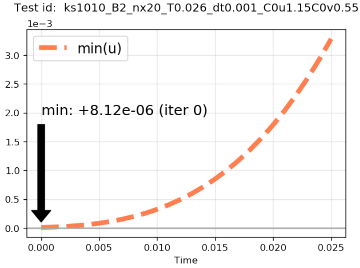
FreeFem++ and LibMesh

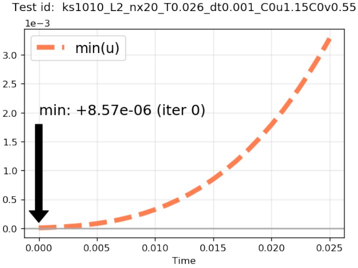
- We used the excellent well-known **FreeFem++** suite for P_1 or P_2 **rapid** & **efficient** software development!
- And also the *C++ FE library* "**LibMesh**"
  - **Open source**, built over other high-quality libraries
  - **Parallel**, using ***PETSc*** or *Trilinos* as linear algebra bakends
  - 1D, 2D, 3D **generic programming**
  - **Variety of Finite Element polynomial families**:
    - Classical P_k-Lagrange
    - Hierarchical high-order Lobatto (order greater than 20)
    - Bernstein positive polynomials
    - Discontinuous P_k
    - ...
  - Element **geometries**: triangles, squares, tetrahedrons
- Other possibilities: DEAL.ii, DUNE, MFEM, FEMPAR (S. Badia et al)...
- Cons and pros: When is the **price of high performance** worth?

P_2 – Bernstein & Lagrange Polynomials

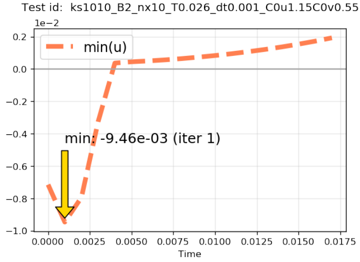
P_2 **Bernstein** Polynomials	P_2 **Lagrange** Polynomials

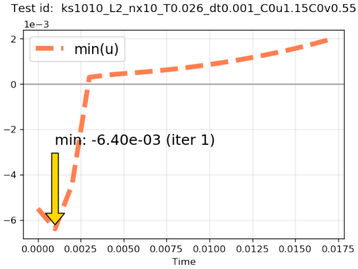
20×20





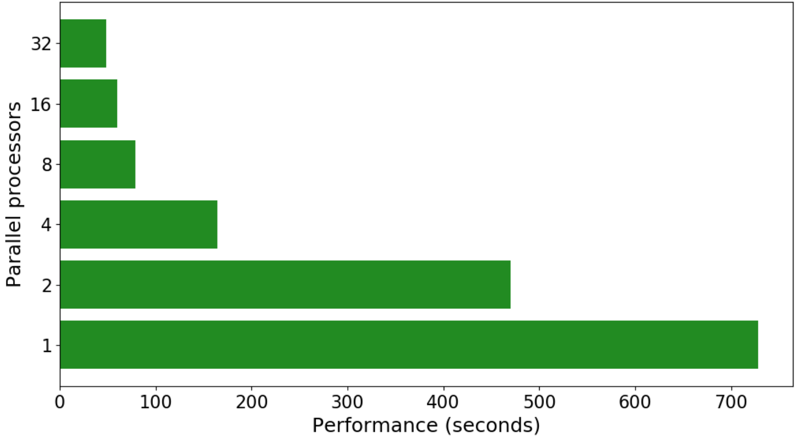
10×10



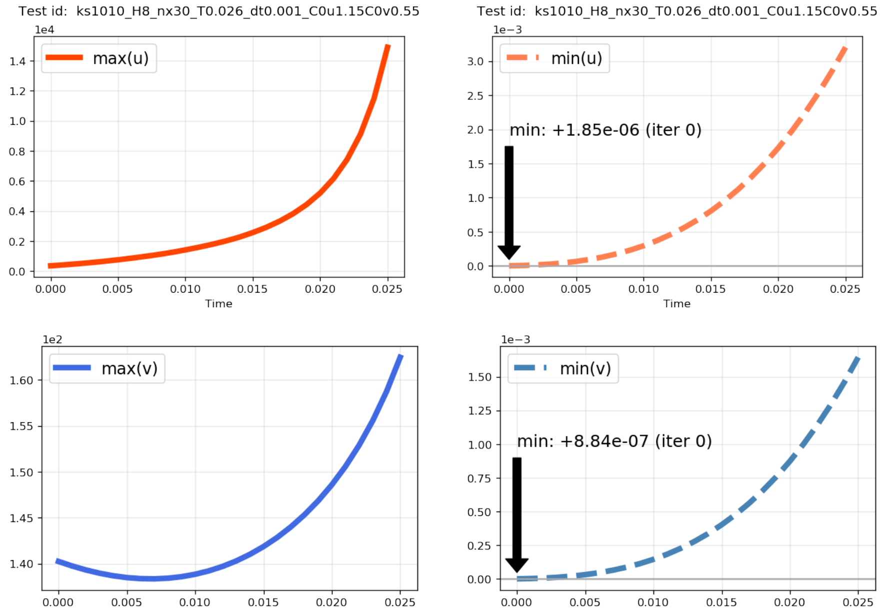


Hierarchical (Lobatto) Order 8 2D FE Test

- We run the following test (using LibMesh in `valle.uca.es`):
  - Time scheme: $S = (1, 0, 1, 0)$, $T_{\text{max}} = 0.026$, $k = 0.001$
  - Space scheme: Lobatto **order 8** polynomial in mesh 30×30
- CPU time for 1, 2, 4,... , 32 processors (7m50s…0m48s):



Results (of Former Test) Are Correct



Section 7

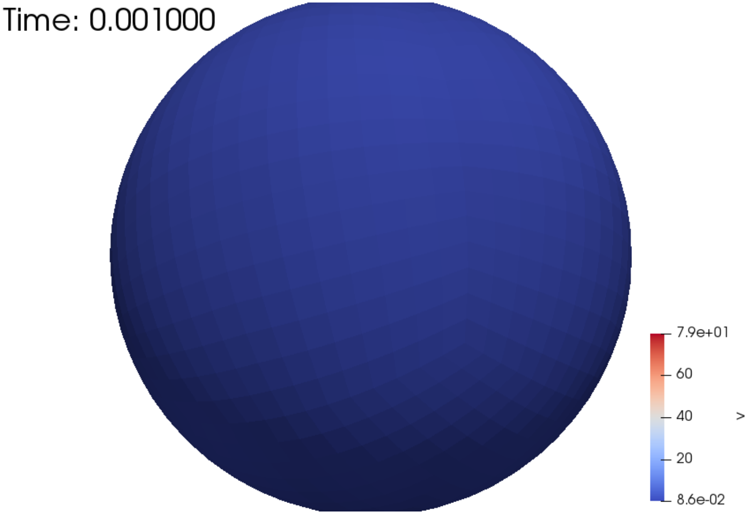
3D Numerical Tests

Classical Keller-Segel 3D Numerical Tests

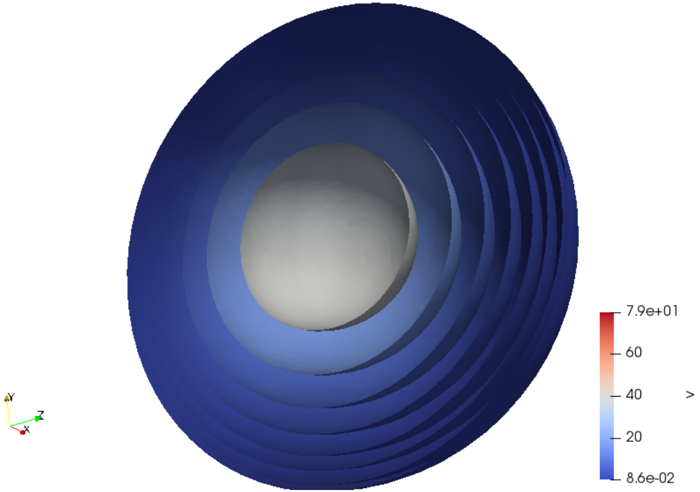
- Now we introduce 3D FE space **discretization**
- LibMesh makes straightforward the **jump "2D $\to$ 3D"**
- **Computing requirements** are much bigger in the 3D case

  $\Rightarrow$ need of parallel computing!
- Playing with initial data, **3D blow up** can easily be obtained...

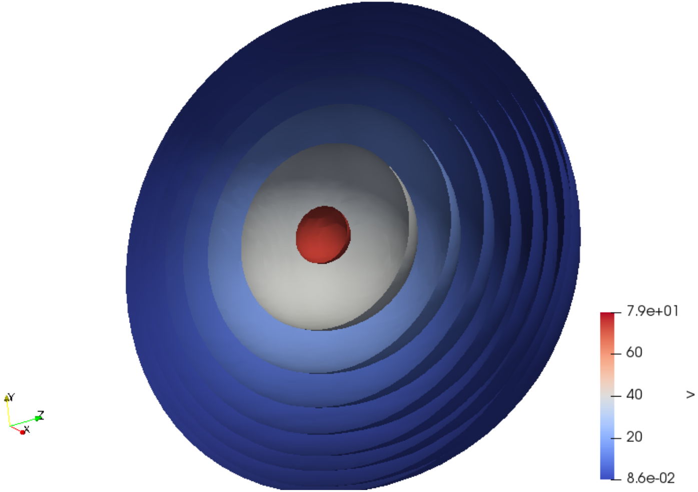
3D Blow-up in a Sphere



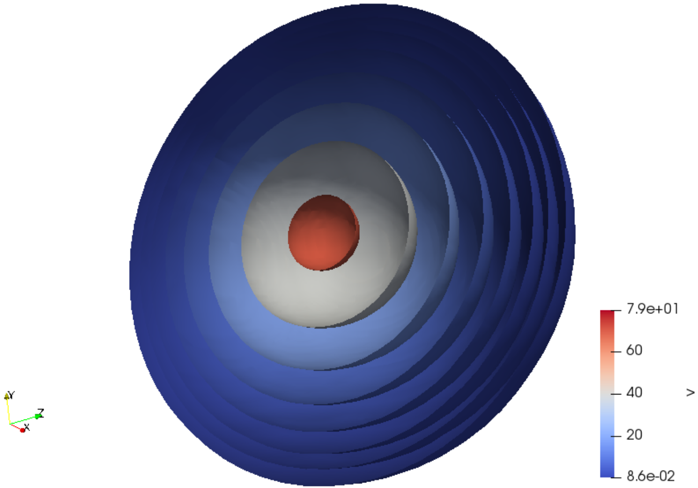
3D Blow-up in a Sphere



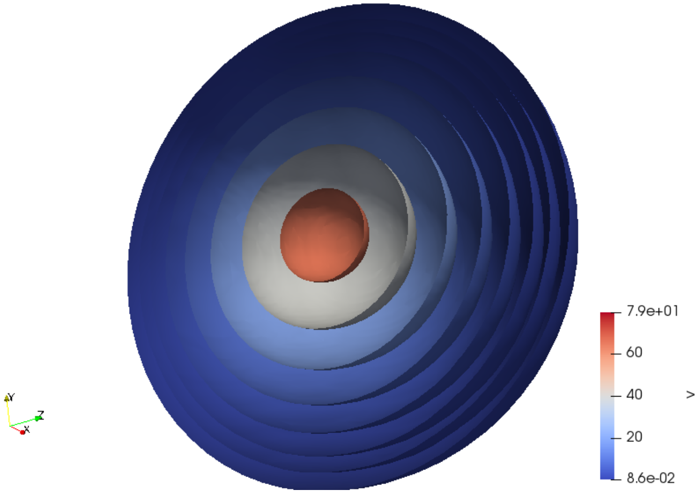
3D Blow-up in a Sphere



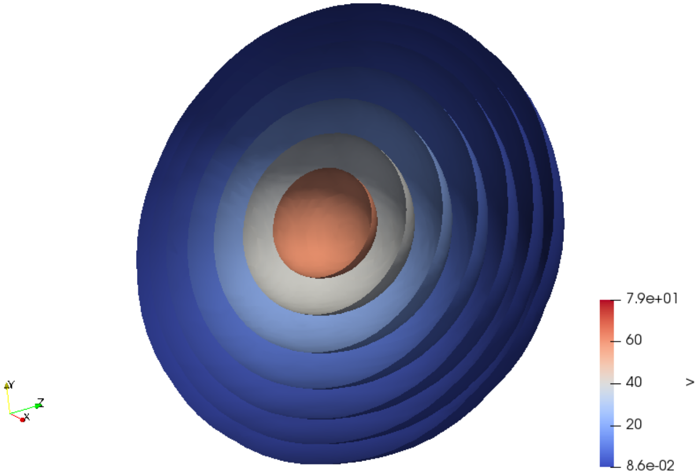
3D Blow-up in a Sphere



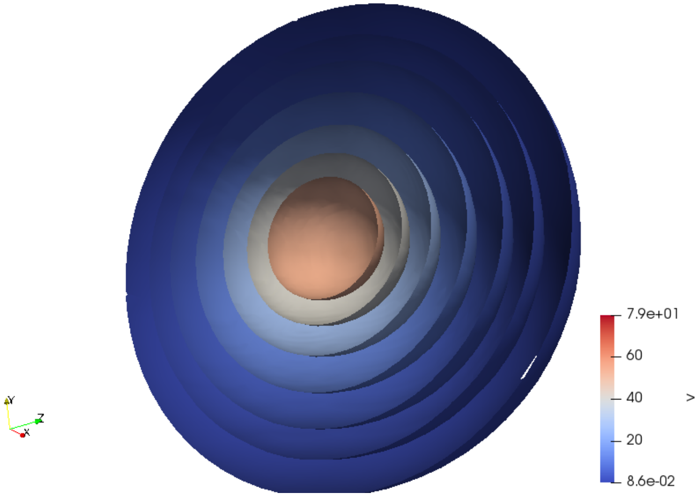
3D Blow-up in a Sphere



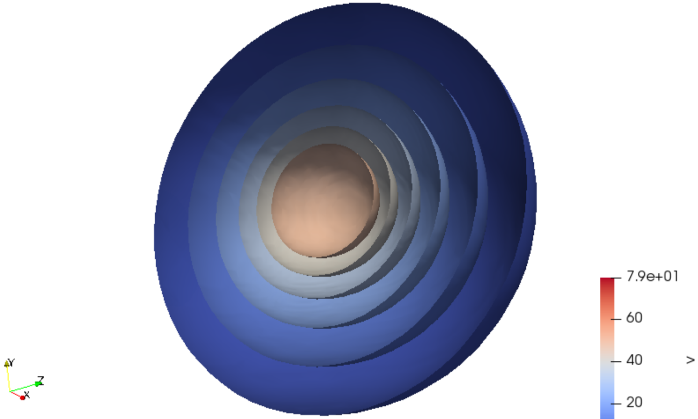
3D Blow-up in a Sphere



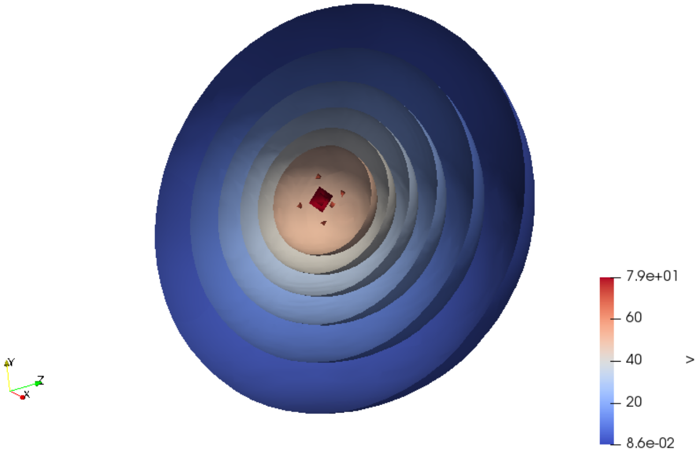
3D Blow-up in a Sphere



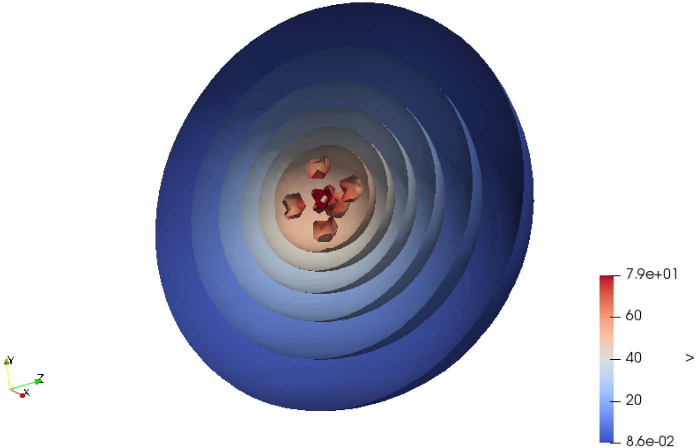
3D Blow-up in a Sphere



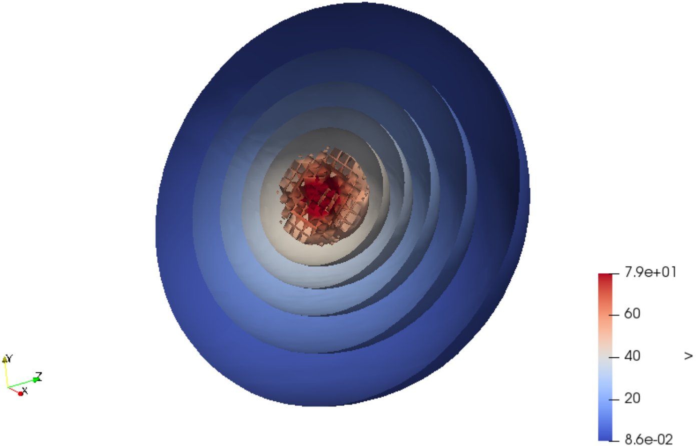
3D Blow-up in a Sphere



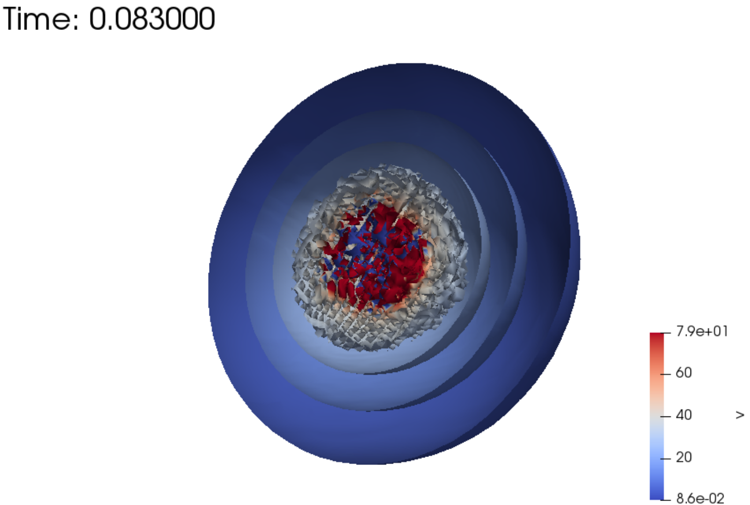
3D Blow-up in a Sphere



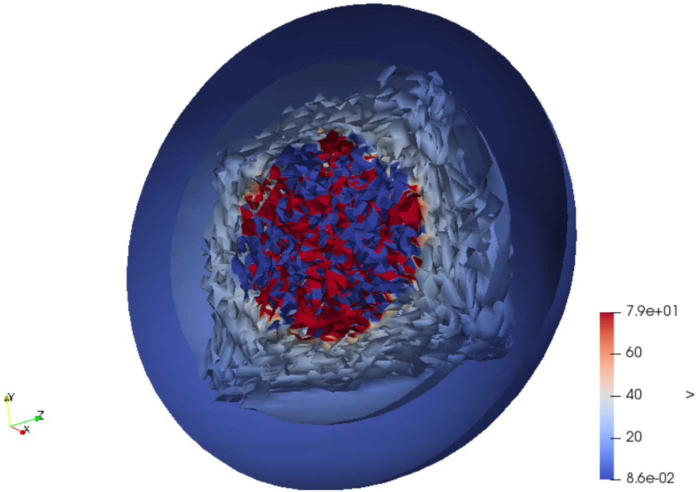
3D Blow-up in a Sphere



3D Blow-up in a Sphere



3D Blow-up in a Sphere



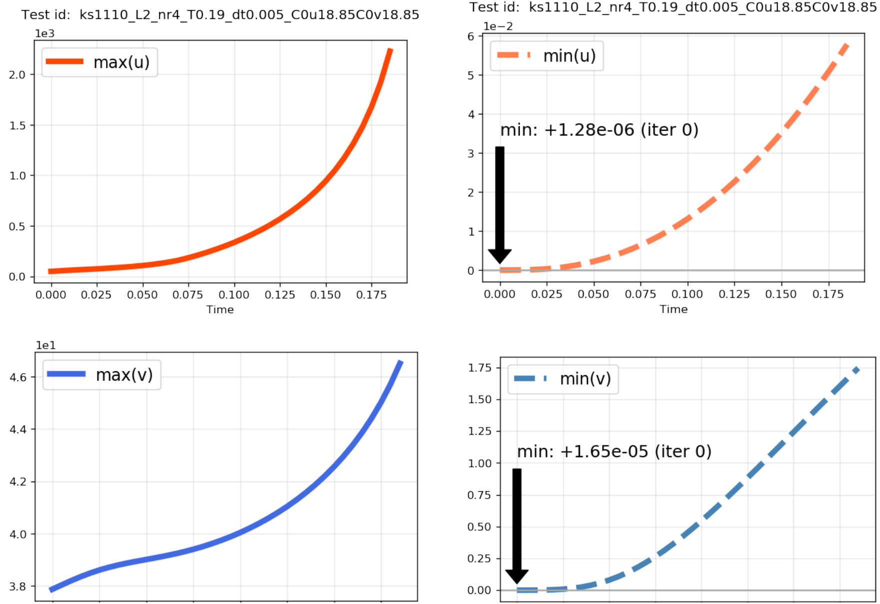
Let us study cases where

blow-up can be avoided for “small initial data”

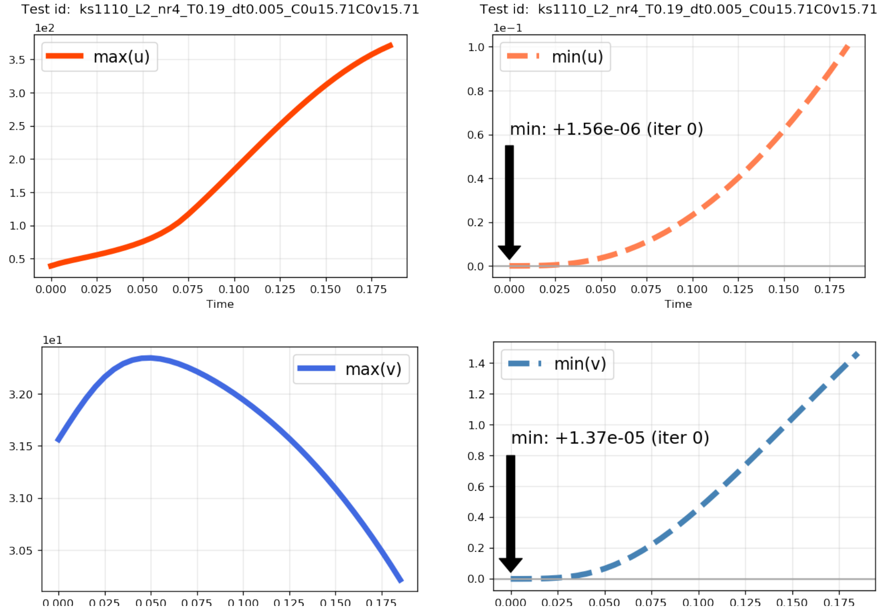
Set of Tests

- $\Omega = \{(x, y, z) \in \mathbb{R}^3 : \; x^2 + y^2 + z^2 < 4\}$
- $(\alpha_0, \alpha_1, \alpha_2, \alpha_3, \alpha_4) = (1, 0.2, 1, 0.1, 1)$ (same parameters than 2D)
- $u_0 = C_u\big(1 + \tanh\big(m_u(1 - x^2 - y^2 - z^2)\big)\big)$, ($\simeq 0$ outside unit sphere)
  $v_0 = C_v\big(1 + \tanh\big(m_v(1 - x^2 - y^2 - z^2)\big)\big)$ (m_u, m_v: initial slope)
- $C_u = C_v = k\,\pi$, with $k \in \mathbb{N}$
- Time discretization: Euler scheme $S = (1, 1, 1, 0)$, $T_{\max} = 0.3$, $k = 0.05$
- Space discretization: P2-Lagrange, $n_r = 4$ refinements from original LibMesh sphere mesh

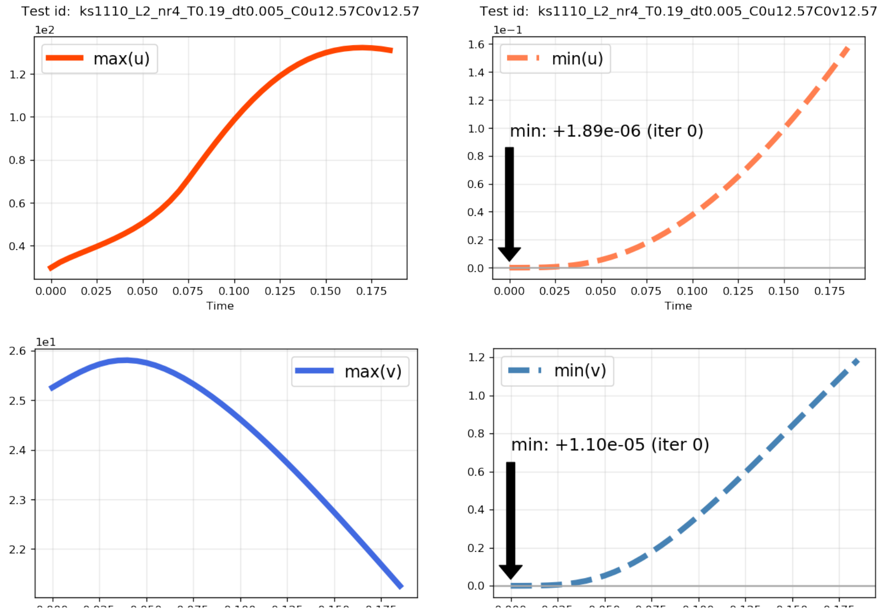
3D Test 1: $C_u = C_v = 6\,\pi$: *Blow Up*



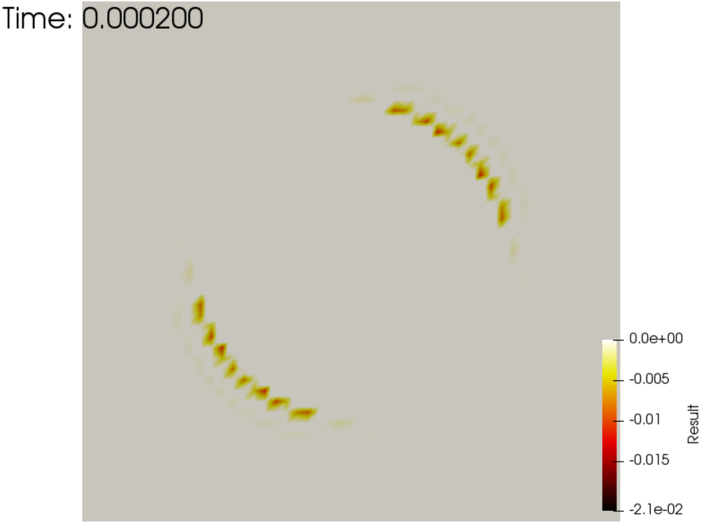
3D Test 2: $C_u = C_v = 5\pi$: *No Blow Up?*



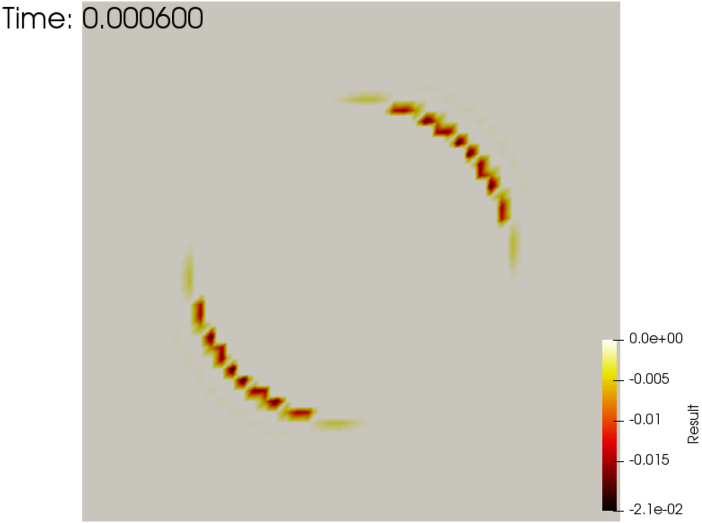
3D Test 3: $C_u = C_v = 4\pi$: **NO Blow Up!**



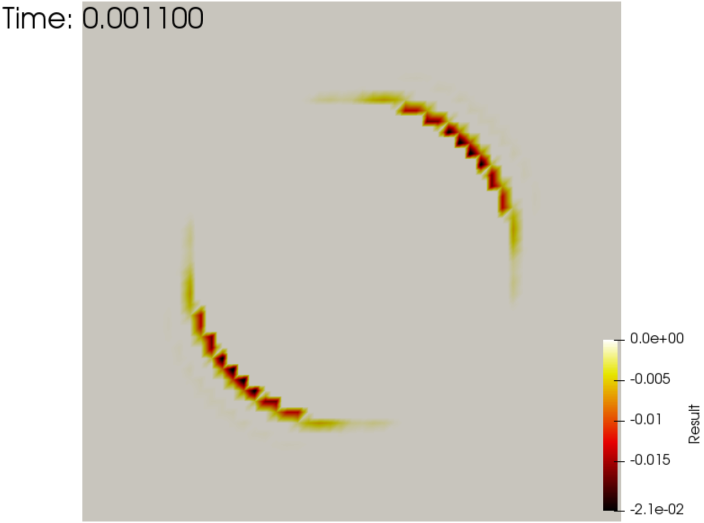
Recent 2D with ideas from 3D initial conditions!



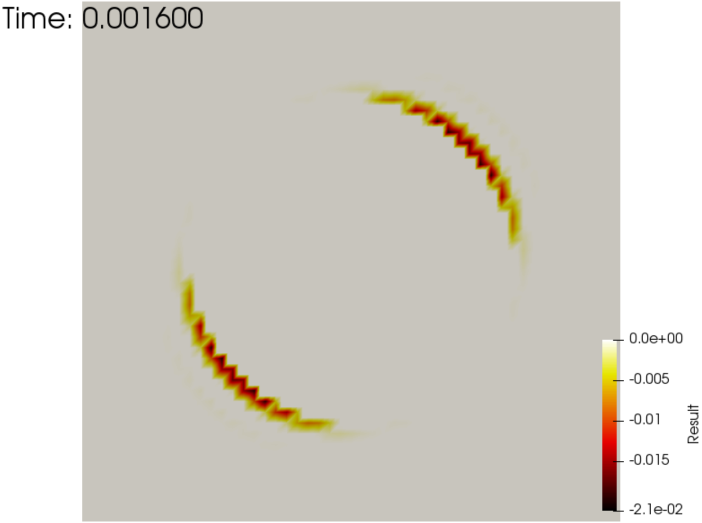
Recent 2D with ideas from 3D initial conditions!



Recent 2D with ideas from 3D initial conditions!



Recent 2D with ideas from 3D initial conditions!



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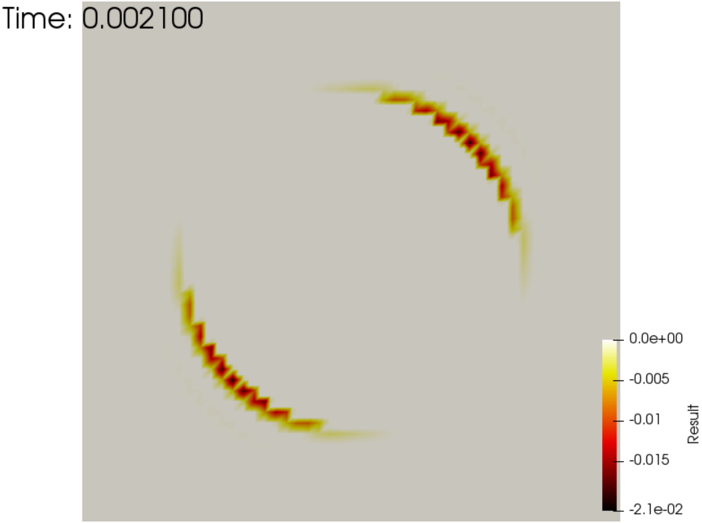

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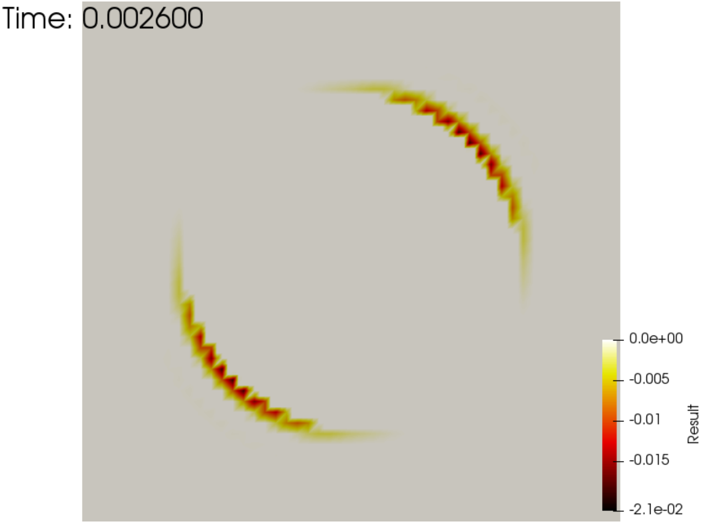

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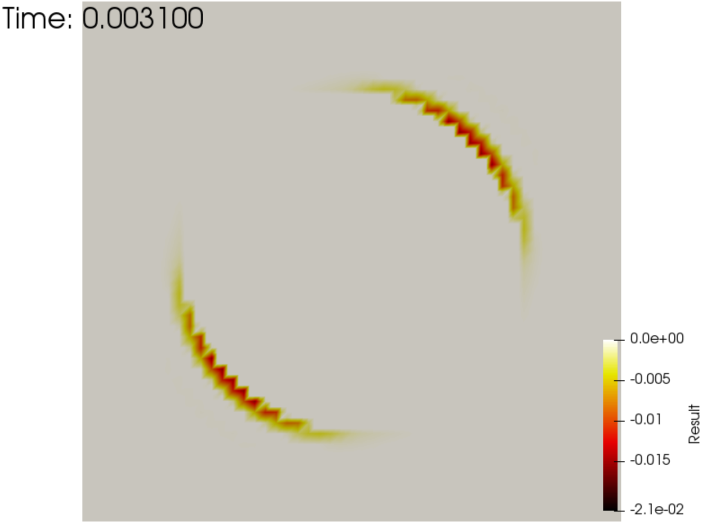

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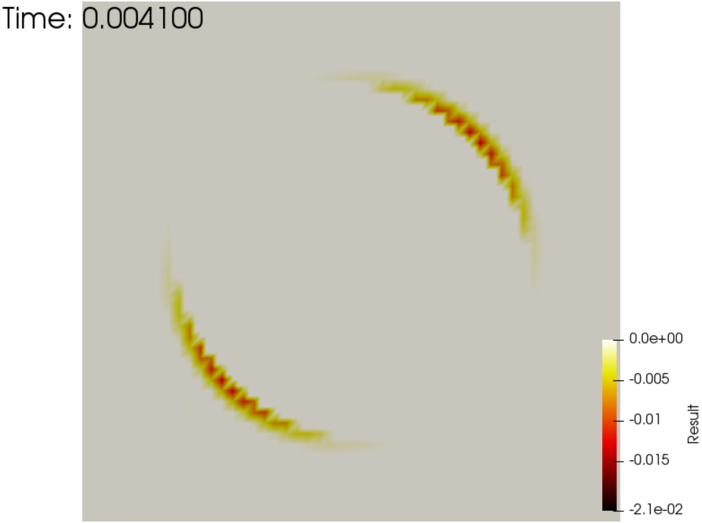

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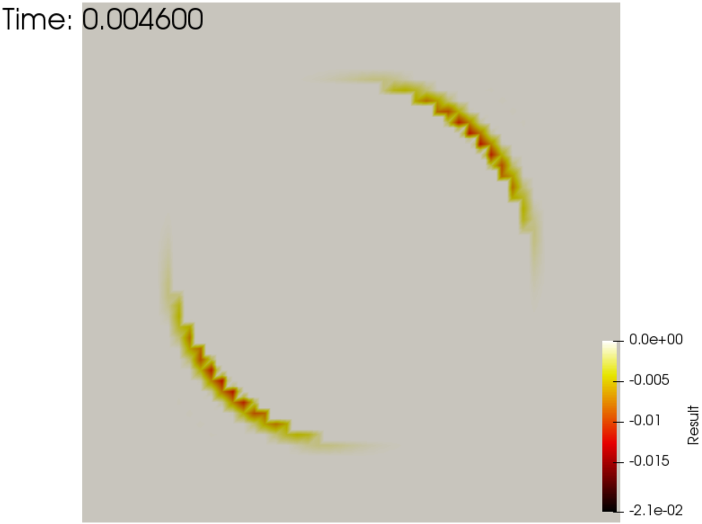

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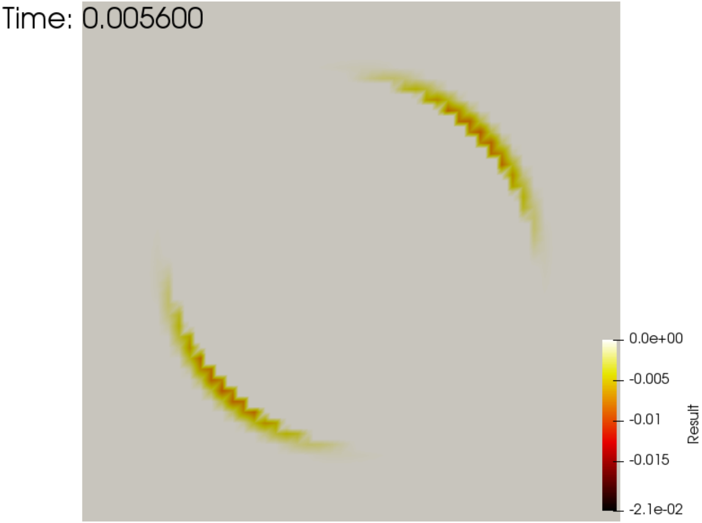

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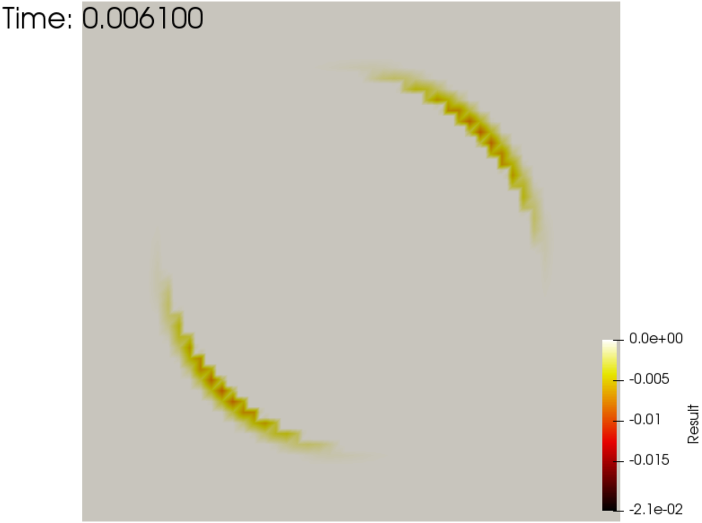

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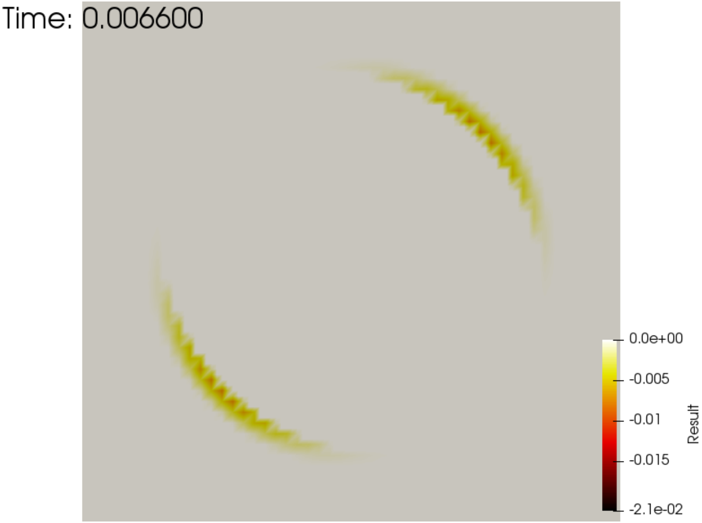

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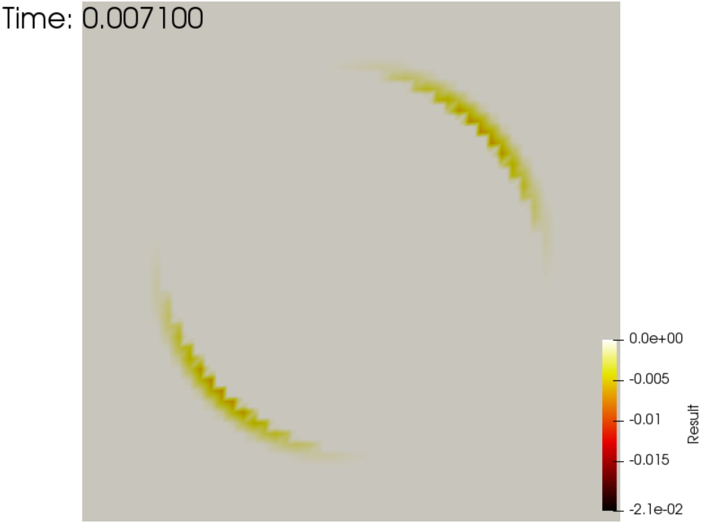

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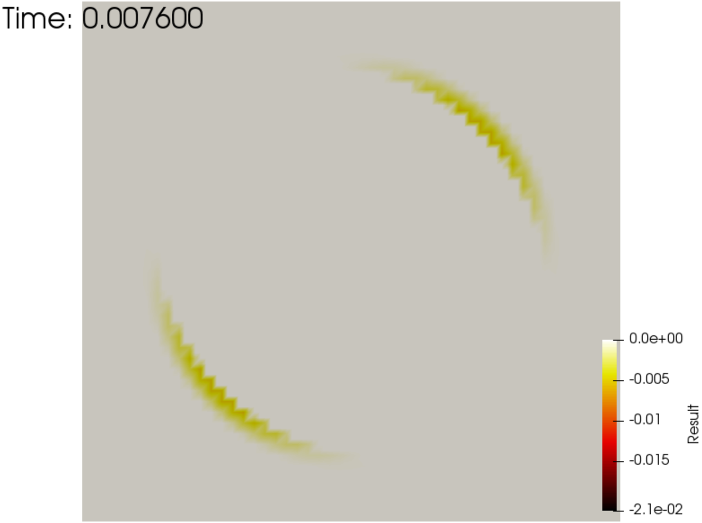

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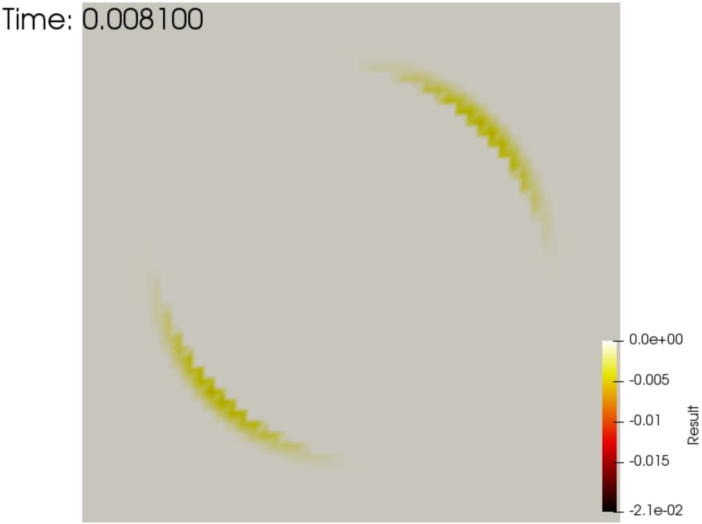

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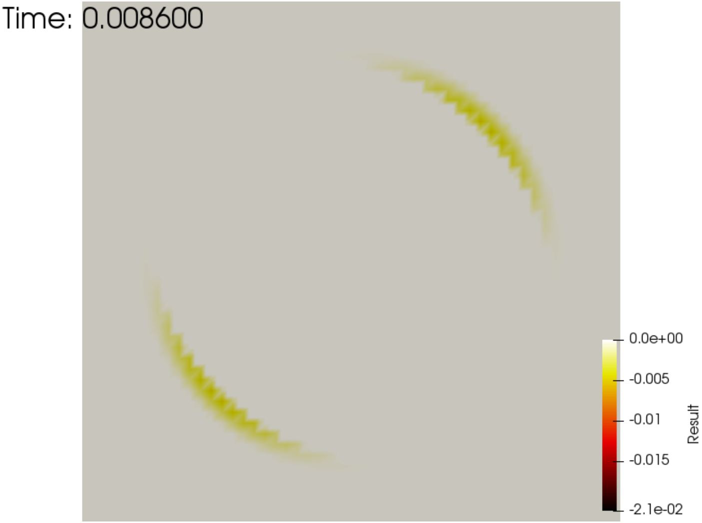

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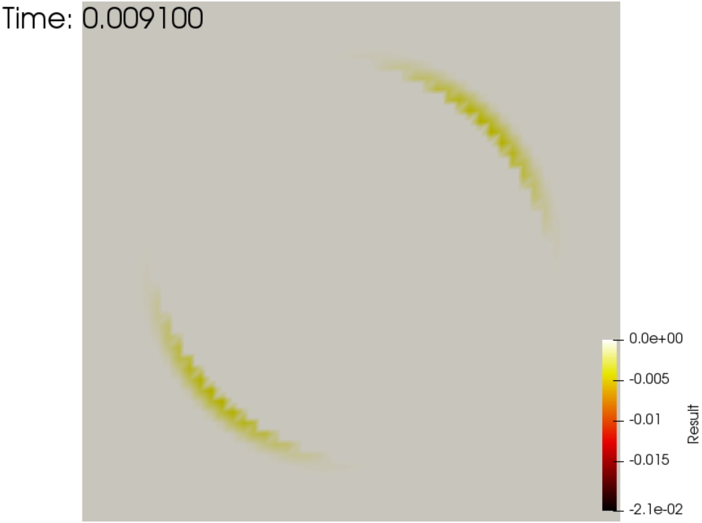

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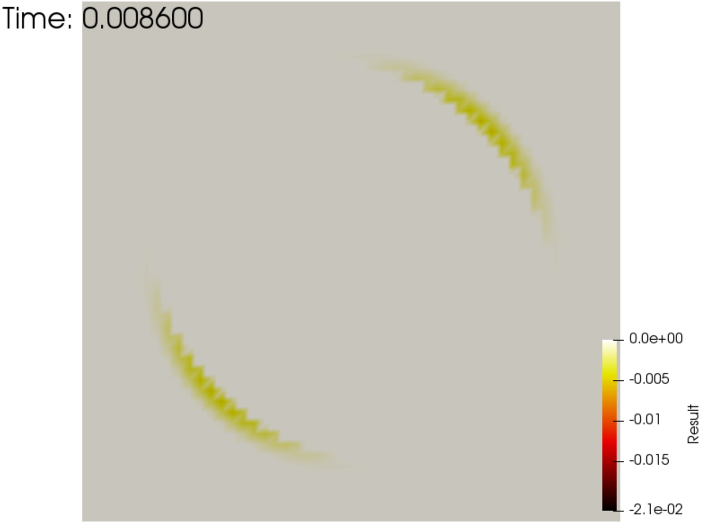

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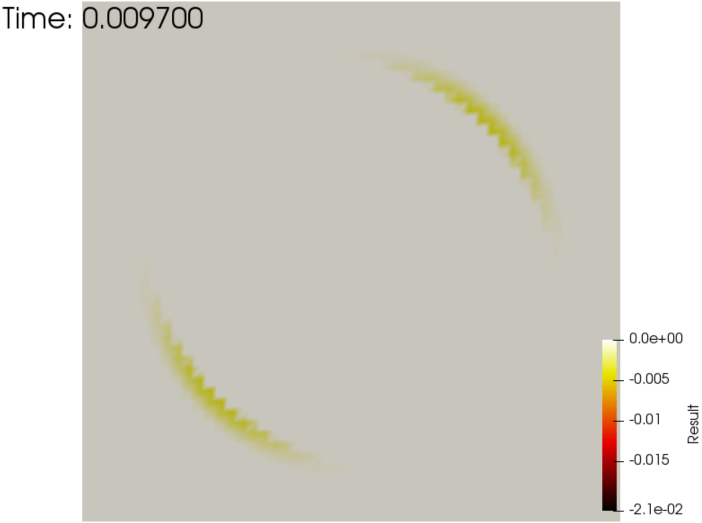

Conclussions

- We got fun in fluid dynamics and classical Keller-Segel numerical simulations
- Very interesting problems, in the **parabolic/hyperbolic** edge!
- In future, lessons from fluids could be applied to Keller-Segel:
  - Try DG and techniques from the hyperbolic world
  - Numerical approximation of blow-up
  - Positivity
  - Other variants of Keller-Segel, coupling with fluids...

¡Muchas gracias!

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Numeric Dissipation and Source Terms

(i,α)	$N_{i,\alpha}$	$F_{i,\alpha}$
$(1,0)$	0	$\frac{k}{2}\int_\Omega \left[\left(\frac{\nabla u^{m+1}}{u^{m+1}}\right)^2 + (\nabla v^{m+1})^2 + 2\big(\delta_t(u^{m+1})\nabla v_{m+r_2}\big)^2\right]$
$(1,1)$	0	0
$(2,0)$	0	$\frac{k}{2}\int_\Omega \left[\left(\frac{u_{m+r_1}}{u^{m+1}}\nabla u^{m+1}\right)^2 + (u_{m+r_1}\nabla v^{m+1})^2 + 2\big(\delta_t(\nabla v^{m+1})\big)^2\right]$
$(2,1)$	0	0
$(3,0)$	0	$\frac{k}{2}\int_\Omega \big(\delta_t(v^{m+1})\big)^2$
$(3,1)$	$\frac{k}{2}\int_\Omega \big(\delta_t(v^{m+1})\big)^2$	0
$(4,0)$	0	0
$(4,1)$	0	$\frac{k}{2}\int_\Omega \left[\big(\delta_t(v^{m+1})\big) + \big(\delta_t(u^{m+1})\big)^2\right]$