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Numbat user's guide

High-resolution simulations of density-driven convective mixing in porous media

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Copyright and disclaimer

Important disclaimer

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Version 9fdce8f, 21/03/2016

1.1 High-resolution simulations of density-driven convective mixing in porous media

Numbat is a massively-parallel code for high-resolution simulations of density-driven convective mixing in porous media built using the MOOSE framework.

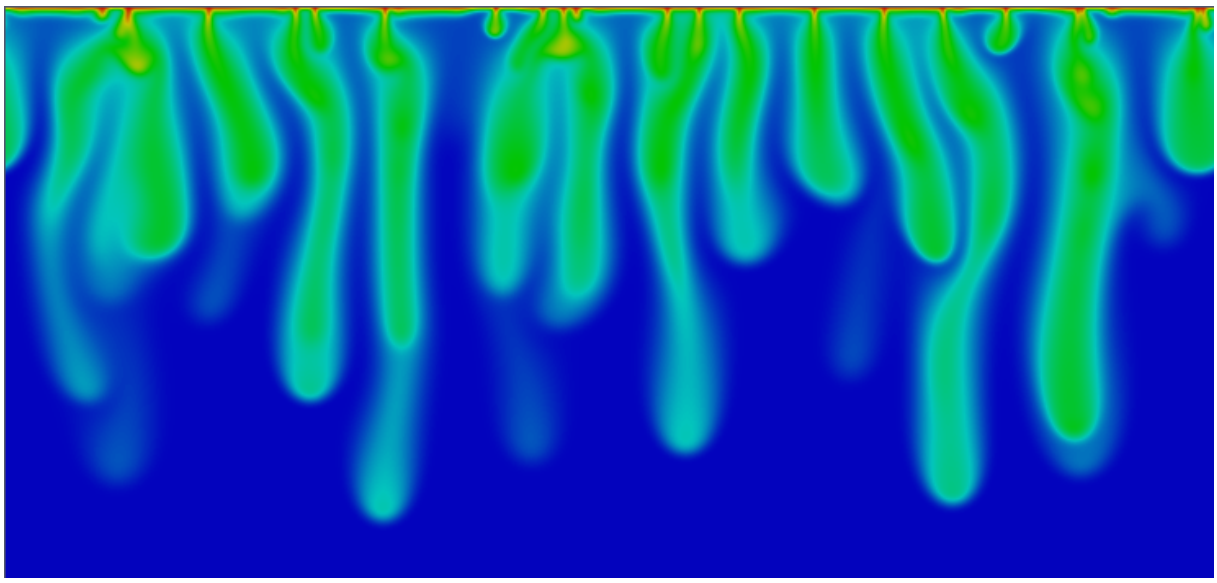

Figure 1.1: Density-driven convective mixing in a porous medium

2 Installation instructions

To install Numbat, follow these simple instructions.

2.1 Install MOOSE

Numbat is based on the MOOSE framework, so the first step is to install MOOSE. For detailed installation instructions depending on your hardware, see www.mooseframework.com.

2.2 Clone Numbat

The next step is to clone the Numbat repository to your local machine.

In the following, it is assumed that MOOSE was installed to the directory *~/projects*. If MOOSE was installed to a different directory, the following instructions must be modified accordingly.

To clone Numbat, use the following commands

```
cd ~/projects
git clone https://github.com/cpgr/numbat.git
cd numbat
git checkout master
```

2.3 Compile Numbat

Next, compile Numbat using

```
make -jn
```

where *n* is the number of processing cores on the computer. If everything has gone well, Numbat should compile without error, producing a binary named *numbat-opt*.

2.4 Test Numbat

Finally, to test that the installation worked, the test suite can be run using

```
./run_tests -jn
```

where *n* is the number of processing cores on the computer.

3 Background theory

3.1 Governing equations

Numbat implements the Boussinesq approximation to model density-driven convective mixing in porous media.

The governing equations for density-driven flow in porous media are Darcy's law

$$\mathbf{u} = -\frac{\mathbf{K}}{\mu}\left(\nabla P + \rho(c) g \hat{\mathbf{k}}\right), \tag{3.1}$$

where $\mathbf{u} = (u, v, w)$ is the velocity vector, $\mathbf{K}$ is permeability, μ is the fluid viscosity, P is the fluid pressure, $\rho(c)$ is the fluid density as a function of solute concentration c, g is gravity, and $\hat{\mathbf{k}}$ is the unit vector in the z direction.

The fluid velocity must also satisfy the continuity equation

$$\nabla \cdot \mathbf{u} = 0, \tag{3.2}$$

and the solute concentration is governed by the convection - diffusion equation

$$\phi \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \phi D \nabla^2 c, \tag{3.3}$$

where ϕ is the porosity, t is time and D is the diffusivity.

Darcy's law and the convection-diffusion equations are coupled through the fluid density, which is given by

$$\rho(c) = \rho_0 + \frac{c}{c_0}\Delta\rho, \tag{3.4}$$

where c_0 is the equilibrium concentration, and $\Delta\rho$ is the increase in density of the fluid at equilibrium concentration.

The boundary conditions are

$$w = 0, \quad z = 0, -H, \tag{3.5}$$

$$\frac{\partial c}{\partial z} = 0, \quad z = -H, \tag{3.6}$$

$$c = c_0, \quad z = 0, \tag{3.7}$$

which correspond to impermeable boundary conditions at the top and bottom boundaries, given by $z = 0$ and $z = -H$, respectively, and a saturated condition at the top boundary.

Initially, there is no solute in the model

$$c = 0, \quad t = 0. \tag{3.8}$$

The governing equations are solved using a streamfunction formulation in 2D and a vector potential formulation in 3D. As a result, we shall consider the two cases separately.

3.2 2D solution

If we consider an anisotropic model, with vertical and horizontal permeabilities given by k_z and k_x, respectively, we can non-dimensionalise the governing equations in 2D following Ennis-King *et. al* (2005). Defining the anisotropy ratio γ as

$$\gamma = \frac{k_z}{k_x}, \tag{3.9}$$

we scale the variables using

$$x = \frac{\phi\mu D}{k_z \Delta\rho g \gamma^{1/2}}\hat{x}, \quad z = \frac{\phi\mu D}{k_z\Delta\rho g}\hat{z}, \quad u = \frac{k_z\Delta\rho g}{\mu\gamma^{1/2}}\hat{u}, \quad w = \frac{k_z\Delta\rho g}{\mu}\hat{w}$$
$$t = \left(\frac{\phi\mu}{k_z\Delta\rho g}\right)^2 \hat{t}, \quad c = c_0\hat{c}, \quad P = \frac{\mu\phi D}{k_z}\hat{P}, \tag{3.10}$$

where $\hat{x}$ refers to a dimensionless variable. The governing equations in dimensionless form are then

$$\mathbf{u} = -\left(\nabla P + c\hat{\mathbf{k}}\right), \tag{3.11}$$
$$\mathbf{u} = 0, \tag{3.12}$$
$$\frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = \gamma\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial z^2}, \tag{3.13}$$

where we have dropped the hat on the dimensionless variables for brevity.

The dimensionless boundary conditions are

$$w = 0, \quad z = 0, -Ra, \tag{3.14}$$
$$\frac{\partial c}{\partial z} = 0, \quad z = -Ra, \tag{3.15}$$
$$c = 1, \quad z = 0, \tag{3.16}$$

where Ra is the Rayleigh number, defined as

$$Ra = \frac{k_z\Delta\rho g H}{\phi\mu D}. \tag{3.17}$$

In this form, the Rayleigh number only appears in the boundary conditions as the location of the lower boundary. Therefore, Ra can be interpreted in this formalism as a dimensionless model height, and can be varied in simulations by simply changing the height of the mesh.

Finally, the dimensionless initial condition is

$$c = 0, \quad t = 0. \tag{3.18}$$

For isotropic models, where $k_x = k_z$ and hence $\gamma = 1$, we recover the dimensionless equations given by Slim (2014).

The coupled governing equations must be solved numerically. To simplify the numerical analysis, we introduce the streamfunction $\psi(x, z, t)$ such that

$$u = -\frac{\partial \psi}{\partial z}, \quad w = \frac{\partial \psi}{\partial x}. \tag{3.19}$$

This definition satisfies the continuity equation, Eq. (3.12), immediately.

The pressure P is removed from Eq. (3.11) by taking the curl of both sides and noting that $\nabla \times \nabla P = 0$ for any P, to give

$$\nabla^2 \psi = -\frac{\partial c}{\partial x}, \tag{3.20}$$

where we have introduced the streamfunction ψ using Eq. (3.19).

The convection-diffusion equation, Eq. (3.13) becomes

$$\frac{\partial c}{\partial t} - \frac{\partial \psi}{\partial z}\frac{\partial c}{\partial x} + \frac{\partial \psi}{\partial x}\frac{\partial c}{\partial z} = \gamma \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial z}. \tag{3.21}$$

The boundary conditions become

$$\frac{\partial \psi}{\partial x} = 0, \quad z = 0, -Ra, \tag{3.22}$$

$$\frac{\partial c}{\partial z} = 0, \quad z = -Ra, \tag{3.23}$$

$$c = 1, \quad z = 0, \tag{3.24}$$

while the initial condition is still given by Eq. (3.18).

In two dimensions, Numbat solves Eq's. (3.20) and (3.21).

3.3 3D solution

We now consider the case of a three-dimensional model. For simplicity, we consider the case where all lateral permeabilities are equal ($k_y = k_x$). The governing equations for the 3D model are identical to the 2D model. In dimensionless form, they are given by Eq's. (3.11) to (3.13), with boundary conditions given by Eq's. (3.14) to (3.16), and initial condition given by Eq. (3.18).

To solve these governing equations in 3D, a different approach must be used as the streamfunction ψ is not defined in three dimensions. Instead, we define a vector potential $\Psi = (\psi_x, \psi_y, \psi_z)$ such that

$$\mathbf{u} = \nabla \times \Psi. \tag{3.25}$$

It is important to note that the vector potential is only known up to the addition of the gradient of a scalar ζ as

$$\nabla \times (\Psi + \nabla \zeta) = \nabla \times \Psi \quad \forall \zeta, \tag{3.26}$$

as $\nabla \times \nabla\zeta = 0$ for any scalar ζ. This uncertainty is referred to as guage freedom, and is common in electrodynamics. Taking the curl of Eq. (3.11) and substituting Eq. (3.25), we have

$$\nabla(\nabla \cdot \Psi) - \nabla^2 \Psi = \left(-\frac{\partial c}{\partial y}, \frac{\partial c}{\partial x}, 0 \right), \tag{3.27}$$

where we have again used the fact that $\nabla \times \nabla P = 0$. If we choose $\nabla \cdot \Psi = 0$ to specify the guage condition, this simplifies to

$$\nabla^2 \Psi = \left(\frac{\partial c}{\partial y}, -\frac{\partial c}{\partial x}, 0 \right). \tag{3.28}$$

As shown in E and Liu (1997), $\nabla \cdot \Psi = 0$ is satisfied throughout the domain if

$$\psi_x = \psi_y = 0, \quad z = 0, -Ra, \quad \frac{\partial \psi_z}{\partial z} = 0, \qquad\qquad z = 0, -Ra.$$

The governing equations are then

$$\nabla^2 \Psi = \left(\frac{\partial c}{\partial y}, -\frac{\partial c}{\partial x}, 0 \right), \tag{3.29}$$

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \gamma \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right) + \frac{\partial^2 c}{\partial z^2}, \tag{3.30}$$

where the continuity is satisfied automatically because $\nabla \cdot (\nabla \times \Psi) = 0$ for any Ψ.

Finally, it is straightforward to show that $\psi_z = 0$ in order to satisfy $\nabla^2 \psi_z = 0$ and $\frac{\partial \psi_z}{\partial z} = 0$, which means that the vector potential has only x and y components,

$$\Psi = (\psi_x, \psi_y, 0), \tag{3.31}$$

and therefore the fluid velocity $\mathbf{u} = (u, v, w)$ is

$$\mathbf{u} = \left(-\frac{\partial \psi_y}{\partial z}, \frac{\partial \psi_x}{\partial z}, \frac{\partial \psi_y}{\partial x} - \frac{\partial \psi_x}{\partial y} \right). \tag{3.32}$$

Note that if there is no y dependence, Eq's. (3.29) and (3.30) reduce to

$$\nabla^2 \Psi = \left(0, -\frac{\partial c}{\partial x}, 0 \right), \tag{3.33}$$

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \gamma \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial z^2}. \tag{3.34}$$

It is simple to show that $\nabla^2 \psi_x = 0$ and $\psi_x = 0$ at $z = 0, -Ra$ are only satisfied if $\psi_x = 0$ in the entire domain. In this case, the governing equations reduce to the two-dimensional formulation, as expected.

In three dimensions, Numbat solves Eq's. (3.29) and (3.30).

4 Input file syntax

The input file for a Numbat simulation is a simple, block-structured text file.

A working example of a 2D problem can be found at https://github.com/cpgr/numbat/blob/master/examples/2D/2Dddc.i

A working example of a 3D problem can be found at https://github.com/cpgr/numbat/blob/master/examples/3D/3Dddc.i

5 Essential input

Details of the minimum input file requirements are given below.

5.1 Mesh

All simulations must feature a mesh. For the basic model with a rectangular mesh, the built-in MOOSE *GeneratedMesh* can be used to create a suitable mesh. In 2D, the input block looks like:

```
[Mesh]
  type = GeneratedMesh
  dim = 2
  xmax = 1000
  ymin = -200
  ymax = 0
  nx = 80
  ny = 20
  bias_y = 0.7
[]
```

This creates a 2D mesh from $x = 0$ to $x = 1000$ and $y = -200$ to $y = 0$ with 80 elements in the x-direction and 20 elements in the y-direction. It is useful to have a mesh that is more refined at the top of the model, to accurately capture the initially small structure of the convective fingers. This is achieved using the built-in *bias_y* parameter.

In 3D, the Mesh block would look like:

```
[Mesh]
  type = GeneratedMesh
  dim = 3
  xmax = 200
  ymax = 200
  zmin = -200
  zmax = 0
  nx = 10
  ny = 10
  nz = 10
  bias_z = 0.7
[]
```

Again, the mesh is refined at the top of the model using the the *bias_z* parameter.

5.2 Variables

For a 2D model, the simulation must have two variables: *concentration* and *streamfunction*. This can be implemented in the input file using the following code:

```
[Variables]
[./concentration]
order = FIRST
family = LAGRANGE
  [./InitialCondition]
    type = PerturbationIC
    variable = concentration
    amplitude = 0.01
    seed = 1
  [../]
[../]
[./streamfunction]
  order = FIRST
  family = LAGRANGE
  initial_condition = 0.0
[../]
[]
```

Initial conditions can also be specified in the *Variables* block. In this case, the initial concentration is perturbed using a *PerturbationIC* to seed the instability.

For a 3D model, three variables are required: one *concentration* variable and two *streamfunction* variables corresponding to the x and y components. This can be implemented in the input file using:

```
[Variables]
  [./concentration]
  [../]
  [./streamfunctionx]
  [../]
  [./streamfunctiony]
  [../]
[]
```

5.3 Kernels

Three kernels are required for a 2D model: a *DarcyDDC* kernel for the *streamfunction* variable, a *ConvectionDiffusionDDC* kernel for the *concentration* variable, and a *TimeDerivative* kernel also for the *concentration* variable. An example for an isotropic model is

```
[Kernels]
  [./TwoDDarcyDDC]
    type = DarcyDDC
    variable = streamfunction
    concentration_variable = concentration
  [../]
```

```
  [./TwoDConvectionDiffusionDDC]
    type = ConvectionDiffusionDDC
    variable = concentration
    streamfunction_variable = streamfunction
    coeff_tensor = '1 0 0 0 1 0 0 0 1'
  [../]
  [./TimeDerivative]
    type = TimeDerivative
    variable = concentration
  [../]
[]
```

The *coeff_tensor* parameter in each convective diffusion kernel can be modified. The format of this

For 3D models, an additional *DarcyDDC* kernel is required for the additional stream function variable. An example of the kernels block for a 3D isotropic model is

```
[Kernels]
  [./ThreeDDarcyDDCx]
    type = DarcyDDC
    variable = streamfunctionx
    concentration_variable = concentration
    component = x
  [../]
  [./ThreeDDarcyDDCy]
    type = DarcyDDC
    variable = streamfunctiony
    concentration_variable = concentration
    component = y
  [../]
  [./ThreeDConvectionDiffusionDDC]
    type = ConvectionDiffusionDDC
    variable = concentration
    streamfunction_variable = 'streamfunctionx streamfunctiony'
    coeff_tensor = '1 0 0 0 1 0 0 0 1'
  [../]
  [./TimeDerivative]
    type = TimeDerivative
    variable = concentration
  [../]
[]
```

In the 3D case, it is important to note that the *DarcyDDC* kernel must specify the component that it applies to, and that the *streamfunction_variable* keyword in the *ConvectionDiffusionDDC* kernel must contain both *streamfunction* variables ordered by the x component then the y component.

5.4 Boundary conditions

Appropriate boundary conditions must be prescribed. Typically, these will be constant concentration at the top of the model domain, periodic boundary conditions on the lateral sides (to mimic an

infinite reservoir), and no-flow boundary conditions at the top and bottom surfaces.

In 2D, this can be achieved using the following input block:

```
[BCs]
  [./conctop]
    type = DirichletBC
    variable = concentration
    boundary = top
    value = 1.0
  [../]
  [./streamfuntop]
    type = DirichletBC
    variable = streamfunction
    boundary = top
    value = 0.0
  [../]
  [./streamfunbottom]
    type = DirichletBC
    variable = streamfunction
    boundary = bottom
    value = 0.0
  [../]
  [./periodic]
    [./x]
      variable = 'concentration streamfunction'
      auto_direction = x
    [../]
  [../]
[]
```

In this case, the *conctop* boundary condition is a Dirichlet condition at the top of the model that fixes the value of concentration to unity. It is useful to note that a MOOSE *GeneratedMesh* provides descriptive names for the sides of the model (top, bottom, left, right) which can be referenced in the input file. No-flow boundary conditions are prescribed on the top and bottom surfaces by holding the *streamfunction* variable constant (in this case 0). Finally, periodic boundary conditions are applied by the *periodic* block, which specifies that both the *concentration* and *streamfunction* variables are periodic on boundaries in the x-direction.

A similar boundary condition block is used in 3D, except that no-flow boundaries must be imposed on both streamfunction variables, see below:

```
[BCs]
  [./conctop]
    type = DirichletBC
    variable = concentration
    boundary = front
    value = 1.0
  [../]
  [./streamfunxtop]
```

```
    type = DirichletBC
    variable = streamfunctionx
    boundary = front
    value = 0.0
  [../]
  [./streamfunxbottom]
    type = DirichletBC
    variable = streamfunctionx
    boundary = back
    value = 0.0
  [../]
  [./streamfunytop]
    type = DirichletBC
    variable = streamfunctiony
    boundary = front
    value = 0.0
  [../]
  [./streamfunybottom]
    type = DirichletBC
    variable = streamfunctiony
    boundary = back
    value = 0.0
  [../]
  [./Periodic]
    [./xy]
      variable = 'concentration streamfunctionx streamfunctiony'
      auto_direction = 'x y'
    [../]
  [../]
[]
```

5.5 Executioner

Each MOOSE simulation must use an *Executioner*, which provides parameters for the solve. In both 2D and 3D models, a transient *Executioner* is used, an example of which is presented below:

```
[Executioner]
  type = Transient
  scheme = bdf2
  dtmin = 0.1
  dtmax = 200
  end_time = 2000
  solve_type = PJFNK
  petsc_options_iname = '-ksp_type -pc_type -pc_sub_type'
  petsc_options_value = 'gmres asm ilu'
  [./TimeStepper]
    type = IterationAdaptiveDT
    dt = 1
```

```
    cutback_factor = 0.5
    growth_factor = 2
  [../]
[]
```

Executioners are a standard MOOSE feature that are well documented on the MOOSE website, so no further detail is provided here.

5.6 Preconditioning

A default preconditioning block is used that provides all Jacobian entries to aid convergence. This is identical for both 2D and 3D models:

```
[Preconditioning]
  [./smp]
    type = SMP
    full = true
  [../]
[]
```

This is a standard MOOSE feature that is documented on the MOOSE website, so no further detail is provided here.

5.7 Outputs

To provide ouptut from the simulation, an *Outputs* block must be specified. An example is

```
[Outputs]
  [./console]
    type = Console
    perf_log = true
    output_nonlinear = true
  [../]
  [./exodus]
    type = Exodus
    file_base = filename
    execute_on = 'INITIAL TIMESTEP_END FINAL'
  [../]
[]
```

In this case, some output regarding the iterations is streamed to the console, while the results are provided in an Exodus file named *filename.e*. There are a large number of output options available in MOOSE, see the MOOSE website for further details.

6 Optional input

While the above required blocks will enable a Numbat simulation to run, there are a number of optional input blocks that will improve the simulations are increase the amount of rsults provided.

6.1 Mesh adaptivity

MOOSE features built-in mesh adaptivity that is extremely useful in Numbat simulations. This can be included using:

```
[Adaptivity]
  marker = combomarker
  max_h_level = 2
  initial_marker = boxmarker
  initial_steps = 1
  [./Indicators]
    [./gradjumpindicator]
      type = GradientJumpIndicator
      variable = concentration
    [../]
  [../]
  [./Markers]
    [./errormarker]
      type = ErrorToleranceMarker
      coarsen = 0.0025
      refine = 0.005
      indicator = gradjumpindicator
    [../]
    [./boxmarker]
      type = BoxMarker
      bottom_left = '0 -1.0 0'
      top_right = '1000 0 0'
      inside = refine
      outside = dont_mark
    [../]
    [./combomarker]
      type = ComboMarker
      markers = 'boxmarker errormarker'
    [../]
  [../]
[]
```

For details about mesh adaptivity, see the MOOSE website.

6.2 Flux at the top boundary

The flux over the top boundary is of particular interest in many cases (especially convective mixing of CO_2). This can be calculated at each time step using a *Postprocessor*:

```
[Postprocessors]
  [./boundaryfluxint]
    type = SideFluxIntegral
    variable = concentration
    boundary = top
    diffusivity = 1
```

```
  [../]
[]
```

The output of the *Postprocessor* can be saved to a *csv* file by including the following additional sub-block in the *Outputs* block:

```
[./csvoutput]
  type = CSV
  file_base = filename
  execute_on = 'INITIAL TIMESTEP_END FINAL'
[../]
```

6.3 Velocity components

The velocity components in the x and y directions (in 2D), and x, y, and z directions in 3D can be calculated using the auxiliary system. These velocity components are calculated using the streamfunction(s), see the governing equations for details.

In the 2D case, two auxiliary variables, u and w, can be defined for the horizontal and vertical velocity components, respectively. Importantly, these auxiliary variables **must** have constant monomial shape functions (these are referred to as *elemental* variables, as the value is constant over each mesh element). This restriction is due to the gradient of the streamfunction variable(s) being undefined for *nodal* auxiliary variables (for example, those using linear Lagrange shape functions). An example of the input syntax for the 2D case is

```
[AuxVariables]
  [./u]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./w]
    order = CONSTANT
    family = MONOMIAL
  [../]
[]
```

For the 3D case, there is an additional horizontal velocity component (v), so the input syntax is

```
[AuxVariables]
  [./u]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./v]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./w]
    order = CONSTANT
```

```
    family = MONOMIAL
  [../]
[]
```

The velocity components are calculated by *VelocityDDCAux* AuxKernels, one for each component. For the 2D case, the input syntax is

```
[AuxKernels]
  [./uAux]
    type = VelocityDDCAux
    variable = u
    component = x
    streamfunction_variable = streamfunction
  [../]
  [./wAux]
    type = VelocityDDCAux
    variable = w
    component = y
    streamfunction_variable = streamfunction
  [../]
[]
```

For the 3D case, three AuxKernels are required. Note that both streamfunction variables must be given, in the correct order (x then y). An example of the input syntax is

```
[AuxKernels]
  [./uAux]
    type = VelocityDDCAux
    variable = u
    component = x
    streamfunction_variable = 'streamfunctionx streamfunctiony'
  [../]
  [./vAux]
    type = VelocityDDCAux
    variable = v
    component = y
    streamfunction_variable = 'streamfunctionx streamfunctiony'
  [../]
  [./wAux]
    type = VelocityDDCAux
    variable = w
    component = z
    streamfunction_variable = 'streamfunctionx streamfunctiony'
  [../]
[]
```

7 2D example

A working example of a 2D problem can be found at https://github.com/cpgr/numbat/blob/master/examples/2D/isotropic/2Dddc.i.

7.1 Input file

The complete input file for this problem is

```
[Mesh]
  type = GeneratedMesh
  dim = 2
  xmax = 1000
  ymin = -200
  ymax = 0
  nx = 80
  ny = 20
  bias_y = 0.7
[]

[Adaptivity]
  marker = combomarker
  max_h_level = 1
  initial_marker = boxmarker
  initial_steps = 1
  [./Indicators]
    [./gradjumpindicator]
      type = GradientJumpIndicator
      variable = concentration
    [../]
  [../]
  [./Markers]
    [./errormarker]
      type = ErrorToleranceMarker
      refine = 0.005
      indicator = gradjumpindicator
    [../]
    [./boxmarker]
      type = BoxMarker
      bottom_left = '0 -1.0 0'
      top_right = '1000 0 0'
      inside = refine
      outside = dont_mark
    [../]
    [./combomarker]
      type = ComboMarker
      markers = 'boxmarker errormarker'
    [../]
  [../]
[]
```

```
[Variables]
  [./concentration]
    order = FIRST
    family = LAGRANGE
    [./InitialCondition]
      type = PerturbationIC
      variable = concentration
      amplitude = 0.02
      seed = 1
    [../]
  [../]
  [./streamfunction]
    order = FIRST
    family = LAGRANGE
    initial_condition = 0.0
  [../]
[]

[Kernels]
  [./TwoDDarcyDDC]
    type = DarcyDDC
    variable = streamfunction
    concentration_variable = concentration
  [../]
  [./TwoDConvectionDiffusionDDC]
    type = ConvectionDiffusionDDC
    variable = concentration
    streamfunction_variable = streamfunction
    coeff_tensor = '1 0 0 0 1 0 0 0 1'
  [../]
  [./TimeDerivative]
    type = TimeDerivative
    variable = concentration
  [../]
[]

[AuxVariables]
  [./u]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./w]
    order = CONSTANT
    family = MONOMIAL
  [../]
[]

[AuxKernels]
```

```
  [./uAux]
    type = VelocityDDCAux
    variable = u
    component = x
    streamfunction_variable = streamfunction
  [../]
  [./wAux]
    type = VelocityDDCAux
    variable = w
    component = y
    streamfunction_variable = streamfunction
  [../]
[]

[BCs]
  [./conctop]
    type = DirichletBC
    variable = concentration
    boundary = top
    value = 1.0
  [../]
  [./streamfuntop]
    type = DirichletBC
    variable = streamfunction
    boundary = top
    value = 0.0
  [../]
  [./streamfunbottom]
    type = DirichletBC
    variable = streamfunction
    boundary = bottom
    value = 0.0
  [../]
  [./Periodic]
    [./x]
      variable = 'concentration streamfunction'
      auto_direction = x
    [../]
  [../]
[]

[Executioner]
  type = Transient
  dtmax = 100
  end_time = 2500
  start_time = 1
  solve_type = PJFNK
  nl_abs_tol = 1e-10
```

```
  [./TimeStepper]
    type = IterationAdaptiveDT
    dt = 1
    cutback_factor = 0.5
    growth_factor = 2
  [../]
  [./TimeIntegrator]
    type = LStableDirk2
  [../]
[]

[Postprocessors]
  [./boundaryfluxint]
    type = SideFluxIntegral
    variable = concentration
    boundary = top
    diffusivity = 1
  [../]
  [./numdofs]
    type = NumDOFs
  [../]
[]

[Preconditioning]
  [./smp]
    type = SMP
    full = true
  [../]
[]

[Outputs]
  [./console]
    type = Console
    perf_log = true
    output_nonlinear = true
  [../]
  [./exodus]
    type = Exodus
    file_base = 2Dddc
    execute_on = 'INITIAL TIMESTEP_END'
  [../]
  [./csvoutput]
    type = CSV
    file_base = 2Dddc
    execute_on = 'INITIAL TIMESTEP_END'
  [../]
[]
```

7.2 Running the example

This example can be run on the commandline using

```
numbat-opt -i 2Dddc.i
```

Alternatively, this file can be run using the *Peacock* gui provided by MOOSE using

```
peacock -i 2Dddc.i
```

in the directory where *2Dddc.i* resides.

7.3 Results

This 2D example should take only a few minutes to run to completion, producing a concentration profile similar to that presented in the following figure, where several downwelling plumes of high concentration can be observed:

Figure 7.1: 2D concentration profile

Note that due to the random perturbation applied to the initial concentration profile, the geometry of the concentration profile obtained will differ from run to run.

The flux over the top boundary is of particular interest in many cases (especially convective mixing of CO_2). This is calculated in this example file using the *boundaryfluxint* postprocessor in the input file, and presented in the following figure

Figure 7.2: 2D flux across the top boundary

Initially, the flux is purely diffusive, and scales as $1/\sqrt{(\pi t)}$, where t is time (shown as the dashed green line). After some time, the convective instability becomes sufficiently strong, at which point the flux across the top boundary rapidly increases (at a time of approximately 1,500 seconds).

8 3D example

A working example of a 3D problem can be found at https://github.com/cpgr/numbat/blob/master/examples/3D/isotropic/3Dddc.i.

8.1 Input file

The complete input file for this problem is

```
[Mesh]
  type = GeneratedMesh
  dim = 3
  xmax = 200
  ymax = 200
  zmin = -200
  zmax = 0
  nx = 10
  ny = 10
  nz = 10
[]

[Adaptivity]
  max_h_level = 2
  initial_marker = boxmarker
  initial_steps = 1
  marker = combomarker
  [./Indicators]
    [./gradjumpindicator]
      type = GradientJumpIndicator
      variable = concentration
    [../]
  [../]
  [./Markers]
    [./errormarker]
      type = ErrorToleranceMarker
      coarsen = 2.5
      refine = 1
      indicator = gradjumpindicator
    [../]
    [./boxmarker]
      type = BoxMarker
      bottom_left = '0 0 -10'
      top_right = '1000 1000 0'
      inside = refine
      outside = dont_mark
    [../]
    [./combomarker]
      type = ComboMarker
      markers = 'boxmarker errormarker'
    [../]
```

```
  [../]
[]

[Variables]
  [./concentration]
    order = FIRST
    family = LAGRANGE
  [../]
  [./streamfunctionx]
    order = FIRST
    family = LAGRANGE
    initial_condition = 0.0
  [../]
  [./streamfunctiony]
    order = FIRST
    family = LAGRANGE
    initial_condition = 0.0
  [../]
[]

[Kernels]
  [./ThreeDDarcyDDCx]
    type = DarcyDDC
    variable = streamfunctionx
    concentration_variable = concentration
    component = x
  [../]
  [./ThreeDDarcyDDCy]
    type = DarcyDDC
    variable = streamfunctiony
    concentration_variable = concentration
    component = y
  [../]
  [./ThreeDConvectionDiffusionDDC]
    type = ConvectionDiffusionDDC
    variable = concentration
    streamfunction_variable = 'streamfunctionx streamfunctiony'
    coeff_tensor = '1 0 0 0 1 0 0 0 1'
  [../]
  [./TimeDerivative]
    type = TimeDerivative
    variable = concentration
  [../]
[]

[AuxVariables]
  [./u]
    order = CONSTANT
```

```
    family = MONOMIAL
  [../]
  [./v]
    order = CONSTANT
    family = MONOMIAL
  [../]
  [./w]
    order = CONSTANT
    family = MONOMIAL
  [../]
[]

[AuxKernels]
  [./uAux]
    type = VelocityDDCAux
    variable = u
    component = x
    streamfunction_variable = 'streamfunctionx streamfunctiony'
  [../]
  [./vAux]
    type = VelocityDDCAux
    variable = v
    component = y
    streamfunction_variable = 'streamfunctionx streamfunctiony'
  [../]
  [./wAux]
    type = VelocityDDCAux
    variable = w
    component = z
    streamfunction_variable = 'streamfunctionx streamfunctiony'
  [../]
[]

[BCs]
  [./conctop]
    type = DirichletBC
    variable = concentration
    boundary = front
    value = 1.0
  [../]
  [./streamfunxtop]
    type = DirichletBC
    variable = streamfunctionx
    boundary = front
    value = 0.0
  [../]
  [./streamfunxbottom]
    type = DirichletBC
    variable = streamfunctionx
```

```
    boundary = back
    value = 0.0
  [../]
  [./streamfunytop]
    type = DirichletBC
    variable = streamfunctiony
    boundary = front
    value = 0.0
  [../]
  [./streamfunybottom]
    type = DirichletBC
    variable = streamfunctiony
    boundary = back
    value = 0.0
  [../]
  [./Periodic]
    [./xy]
      variable = 'concentration streamfunctionx streamfunctiony'
      auto_direction = 'x y'
    [../]
  [../]
[]

[Preconditioning]
  [./smp]
    type = SMP
    full = true
  [../]
[]

[Executioner]
  type = Transient
  scheme = bdf2
  dtmin = 0.1
  dtmax = 1000
  end_time = 3000
  solve_type = PJFNK
  petsc_options_iname = '-pc_type -sub_pc_type -pc_asm_overlap'
  petsc_options_value = 'asm ilu 4'
  [./TimeStepper]
    type = IterationAdaptiveDT
    dt = 1
  [../]
[]

[Postprocessors]
  [./boundaryfluxint]
    type = SideFluxIntegral
    variable = concentration
```

```
    boundary = front
    diffusivity = 1
  [../]
  [./numdofs]
    type = NumDOFs
  [../]
[]

[Outputs]
  output_initial = true
  [./console]
    type = Console
    perf_log = true
    output_nonlinear = true
    output_linear = true
  [../]
  [./exodus]
    type = Exodus
    file_base = 3Dddc
    execute_on = 'INITIAL TIMESTEP_END'
  [../]
  [./csvoutput]
    type = CSV
    file_base = 3Dddc
    execute_on = 'INITIAL TIMESTEP_END'
  [../]
[]
```

8.2 Running the example

Note: This example should **not** be run on a laptop or workstation due to the large computational requirements. Do not run this using the *Peacock* gui provided by MOOSE.

Running this example on a cluster results in total run times of over 27 hours for a single processor down to only 30 minutes using 100 processors in parallel.

8.3 Results

This 3D example should produce a concentration profile similar to that presented in the following figure, where several downwelling plumes of high concentration can be observed:

Figure 8.1: 3D concentration profile

Note that due to the random perturbation applied to the initial concentration profile, the geometry of the concentration profile obtained will differ from run to run.

The flux over the top surface is of particular interest in many cases (especially convective mixing of CO_2). This is calculated in this example file using the *boundaryfluxint* postprocessor in the input file, and presented in the following figure

Figure 8.2: 3D flux across the top boundary

Initially, the flux is purely diffusive, and scales as $1/\sqrt{(\pi t)}$, where t is time (shown as the dashed green line). After some time, the convective instability becomes sufficiently strong, at which point the flux across the top boundary rapidly increases (at a time of approximately 1,700 seconds). Also shown for comparison is the flux for the 2D example. It is apparent that the 3D model leads in a slower onset of convection (the time where the flux first increases from the diffusive rate).

9 References

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