TP2: Poisson's equation

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TC5 : TPs sur les méthodes numériques et simulations
Séances du 18 et 22 novembre 2019 à Jussieu

Outline

- For which plasma studies do we need to solve Poisson's equation and not Maxwell equations?
- Work to be done

For which plasma studies do we need to solve Poisson's equation?

For low-temperature plasmas:

- Electrostatic Particle-In-Cell (PIC) simulations for low-pressure plasmas
- Fluid simulations of low-temperature plasmas at atmospheric pressure

$\rightarrow$ back-up slides for details

Outline

- For which plasma studies do we need to solve Poisson's equation?
- Work to be done : Solve Poisson's equation in 1D and then in 2D

Poisson's equation

$$\varepsilon_0 \nabla \cdot (\varepsilon_r \nabla V) = -q_e(n_p - n_n - n_e)$$

In this work, the source term will be defined as ρ

$$\varepsilon_0 \nabla \cdot (\varepsilon_r \nabla V) = -\rho$$

We propose the following exercices:

- Exercice 1 : 1D poisson solver for a plasma between metallic walls ($\varepsilon_r = 1$)
- Exercice 2 : 1D poisson solver: performances
- Exercice 3 : 2D poisson solver for a plasma between metallic walls
- Exercice 4 (optional) : 1D poisson solver for a plasma between metallic walls covered by dielectric walls

Poisson's equation in 1D

In 1D:

$$\varepsilon_0 \nabla_x \cdot (\varepsilon_\mathrm{r} \nabla_x V(x)) = -\rho(x)$$

For the numerical integration : we propose to use a finite volume approach. This approach is conservative
In 1D for a uniform mesh finite volume, and finite difference approaches give the same discretized form.

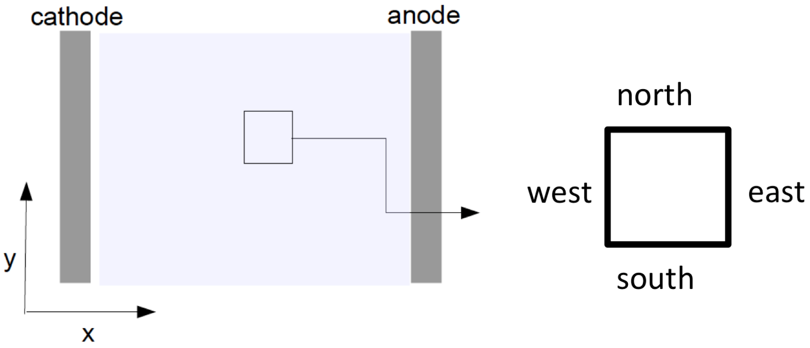
Mesh in 1D

- We discretize the domain $x = [0, Lx]$ in $N - 2$ cells of size dx and 2 half-cells
- The center of each cell is defined by the index i
- The unknown potential $V(x)$ becomes V_i and the source term $\rho(x)$ becomes ρ_i
- The unknowns are mean values at the center of cells
- The center of the cell $i = 1$ correspond to $x = 0$, and $i = N$ corresponds to $x = L_x$

$\rightarrow$ exercices 1 and 2

Exercice 3 : Finite volume method in 2D

Volume of the discharge = $\sum$ elementary cells



Exercice 3 : Integration of Poisson's equation in 2D

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_\mathrm{r} \boldsymbol{\nabla} V) = -\rho \tag{1}$$

Poisson's equation can be written as :

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = -\rho \tag{2}$$

with

$$\boldsymbol{D} = -\varepsilon_0 \varepsilon_\mathrm{r} \boldsymbol{\nabla} V = \varepsilon_0 \varepsilon_\mathrm{r} \boldsymbol{E} \tag{3}$$

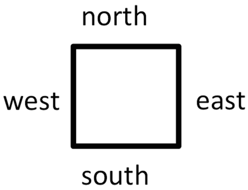
Exercice 3 : Integration of Poisson's equation in 2D

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = -\rho \tag{4}$$

$$\iiint\limits_{V_c} \boldsymbol{\nabla} \cdot \boldsymbol{D} dV = - \iiint\limits_{V_c} \rho dV \tag{5}$$

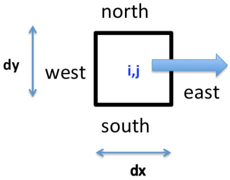
$$\oint\!\!\!\oint\limits_{S} \boldsymbol{D} \cdot \boldsymbol{dS} = -\bar{\rho} V_c \tag{6}$$

$$\frac{1}{V_c} \sum_{f} D_{Nf} \cdot S_f = -\bar{\rho} \tag{7}$$



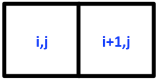
Exercice 3 : Integration of Poisson's equation in 2D

As an example: the EAST interface



$$\frac{D_{Ne} S_{fe}}{V_c} = \frac{1}{dx.dy} \epsilon_0 \epsilon_r E_{Ne} dy$$

As $\epsilon_r = 1$ and the mesh is uniform:



$$E_{Ne} = -\frac{V_{i+1} - V_i}{dx}$$

Exercice 3 : Integration of Poisson's equation in 2D on a control volume

In doing the same on all interfaces, we obtain:

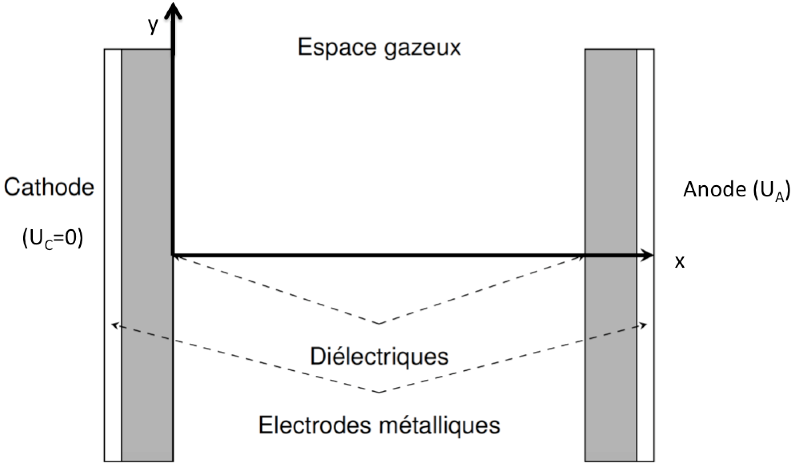
$$Ve_{i,j}.V_{i+1,j} + Vw_{i,j}.V_{i-1,j} + Vn_{i,j}.V_{i,j+1} + Vs_{i,j}.V_{i,j-1} - Vc_{i,j}.V_{i,j} = -\rho_{i,j} \quad (8)$$

where

$$Vc_{i,j} = Ve_{i,j} + Vw_{i,j} + Vn_{i,j} + Vs_{i,j} \quad (9)$$

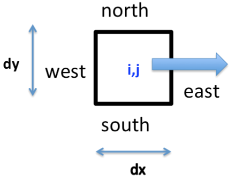
In 2D : The coefficients Ve,Vw,Vn and Vs are known : how to calculate $V_{i,j}$?
$\rightarrow$ exercice 3

Exercice 4 : Studied configuration:

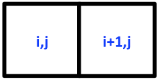


Exercice 4 : Integration of Poisson's equation with a permittivity that may vary from one cell to another

As an example: the EAST interface



$$\frac{D_{Ne} S_{fe}}{V_c} = \frac{1}{dx.dy} \epsilon_{i,j} E_{Ne} dy \quad (10)$$

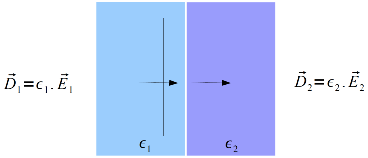


with $\epsilon = \epsilon_0 \epsilon_r(x, y)$

$$E_{Ne} = -\frac{V_{i+1/2} - V_i}{dx/2} \quad (11)$$

Exercice 4 : Integration of Poisson's equation on a control volume

Case of the interface of two materials with different dielectric properties:
The mesh is done such that the interface between materials corresponds to an interface between cells



$$\iiint_V \nabla \cdot \boldsymbol{D} dV = -\iiint_V \rho dV \tag{12}$$

$$\oiint_S \boldsymbol{D} \cdot \boldsymbol{dS} = -\bar{\rho} V \tag{13}$$

with no surface charges on the dielectric surface

$$D_{N1} = D_{N2} \tag{14}$$

Exercice 4 : Integration of Poisson's equation on a control volume

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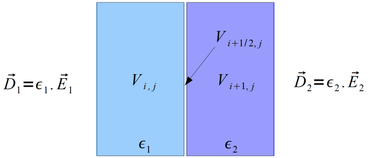


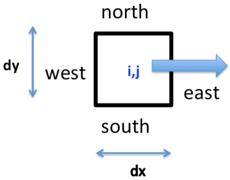
$$D_{N1} = D_{N2} \quad (15)$$

$$\epsilon_i \frac{V_{i+1/2} - V_i}{dx/2} = \epsilon_{i+1} \frac{V_{i+1} - V_{i+1/2}}{dx/2} \quad (16)$$

$$V_{i+1/2} = \frac{\epsilon_{i+1}}{\epsilon_i + \epsilon_{i+1}} V_{i+1} + \frac{\epsilon_i}{\epsilon_i + \epsilon_{i+1}} V_i \quad (17)$$

Exercice 4 : Integration of Poisson's equation on a control volume

As an example: the EAST interface



$$\frac{D_{Ne}S_{fe}}{V_c} = \frac{1}{dx.dy}\epsilon_{i,j}E_{Ne}dy \qquad (18)$$

$$E_{Ne} = -\frac{V_{i+1/2,j} - V_{i,j}}{dx/2} = -\frac{2\epsilon_{i+1,j}(V_{i+1,j} - V_{i,j})}{dx(\epsilon_{i,j} + \epsilon_{i+1,j})} \qquad (19)$$

$$\frac{D_{Ne}S_{fe}}{V_c} = -\frac{2\epsilon_{i,j}\epsilon_{i+1,j}}{dx^2(\epsilon_{i,j} + \epsilon_{i+1,j})}(V_{i+1,j} - V_{i,j}) \qquad (20)$$

Exercice 4 : Integration of Poisson's equation on a control volume

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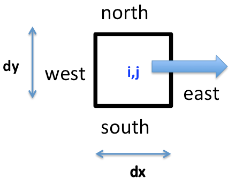

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$$E_{Ne} = -\frac{V_{i+1/2,j} - V_{i,j}}{dx/2} = -\frac{2\epsilon_{i+1,j}(V_{i+1,j} - V_{i,j})}{dx(\epsilon_{i,j} + \epsilon_{i+1,j})} \tag{19}$$

$$\frac{D_{Ne} S_{fe}}{V_c} = \underbrace{-\frac{2\epsilon_{i,j}\epsilon_{i+1,j}}{dx^2(\epsilon_{i,j} + \epsilon_{i+1,j})}}_{Ve_{i,j}} (V_{i+1,j} - V_{i,j}) \tag{20}$$

back-up slides

For which plasma studies do we need to solve Poisson's equation?

For low-temperature plasmas:

- Electrostatic Particle-In-Cell (PIC) simulations for low-pressure plasmas with static magnetic fields
- Non magnetized plasmas : Fluid simulations of low-temperature plasmas at atmospheric pressure

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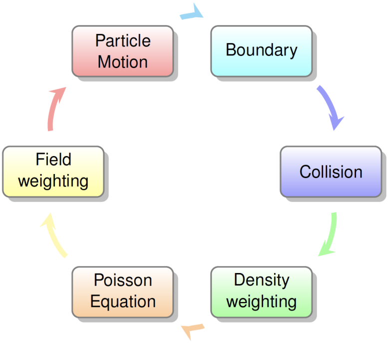
Electrostatic PIC simulations for low-temperature plasmas at low pressure

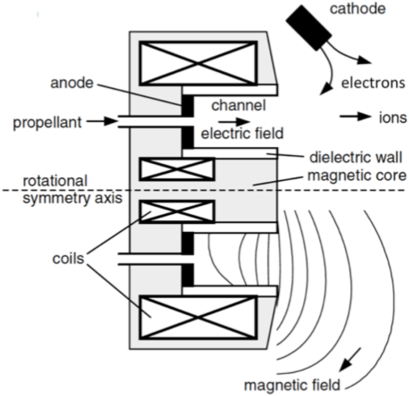
Standard Particle in Cell simulation:

- Explicit
- Electrostatic
- Numerous gases
  - Helium
  - Argon
  - Krypton
  - Xenon



Example : Electrostatic PIC simulations for electric propulsion applications

Figure: Example of HET - PPS© 1350 Safran



Hall effect thruster (HET) :
A low-temperature low-pressure plasma with a fixed magnetic field
Plasma interaction with dielectric walls

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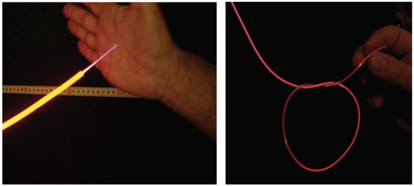
What is a low-temperature plasma at P_{atm} ?

- Electron density $\ll$ neutral density : ionization degree of about 10^{-4}-10^{-5}
- T_e (10 000 to 50 000 K) $\gg$ T_N=300 K
- Interest of low-temperature plasmas at P_{atm}: nonequilibrium chemistry at room temperature

Non-thermal discharges at atmospheric pressure

Applications of non-thermal discharges at P_{atm} ?

- Since a few years, many studies on non-thermal discharges at atmospheric ground pressure
- Wide range of applications at low pressure → possible at ground pressure to reduce costs (no need for pumping systems) ?
- New applications as biomedical applications, plasma assisted combustion



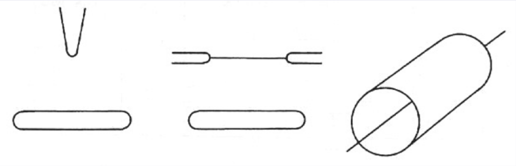
Robert *et al.*, Plasma Process. Polym. 2009, 6, 795-802

G. Pilla, PhD thesis (2008)

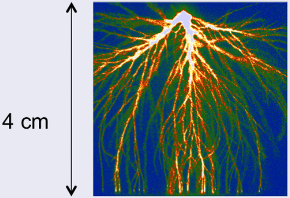
How to generate non-thermal discharges at atmospheric pressure ?

Between two metallic electrodes

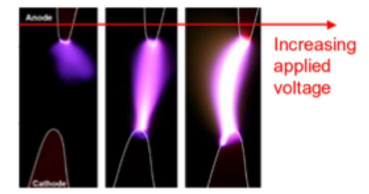
- Interelectrode gaps of a few mm to a few cm at P_{atm}



- If the gap distance > 1cm → complex discharge structure



Briels, PhD (2007)



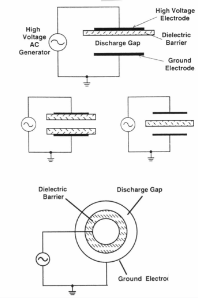
Pai, D., 2008 Ph.D. thesis, Ecole Centrale Paris, France.

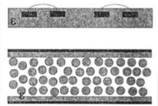
- Risk: If the voltage pulse is too long → transition to spark (thermal plasma!)

How to generate non-thermal discharges at atmospheric pressure ?

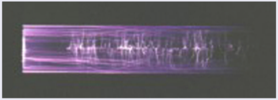
Dielectric Barrier Discharge (DBD)

- Interelectrode gaps of a few mm to a few cm at P_{atm}

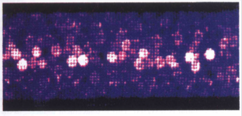




Plane-plane reactor (LPGP Orsay)



Wire-cylinder (GREMI Orléans)

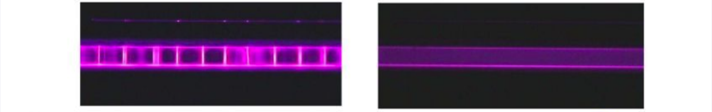


H.Russ et al , *IEEE Trans. Plasma Sci.* **27** (1999) 38

Non-thermal discharges at atmospheric pressure

Structure of P_{atm} discharges

- At P_{atm}, non-thermal atmospheric pressure discharges may have filamentary or diffuse structures



Filamentary discharges: most frequent

- High electron density (10^{14} cm^{-3}) in a filament with a radius of the order of 100 μm $\rightarrow$ high density of active species (radicals, excited species). In some cases, local heating may occur

Diffuse discharges

- Low density of electrons, large volume of the discharge and negligible heating

Simplest 2D Fluid model for discharge in air at $\mathrm{P_{atm}}$

- Continuity equation is solved for electrons, positive and negative ions

$$\frac{\partial n_i}{\partial t} + \mathrm{div}\, \boldsymbol{j}_i = S_i \tag{21}$$

- Drift-diffusion approximation

$$\boldsymbol{j}_i = \mu_i \, n_i \, \boldsymbol{E} - D_i \, \mathbf{grad} \, n_i \tag{22}$$

- Poisson's equation:

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_\mathrm{r} \boldsymbol{\nabla} V) = -q_\mathrm{e}(n_\mathrm{p} - n_\mathrm{n} - n_\mathrm{e}) \tag{23}$$

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- Strong non-linear coupling between drift-diffusion and Poisson's equations
- The species densities have to be calculated accurately as their difference is used to compute the potential and then the electric field $\rightarrow$ crucial to simulate the propagation of ionization fronts

- Continuity equation is solved for electrons, positive and negative ions

$$\frac{\partial n_i}{\partial t} + \mathrm{div}\, \boldsymbol{j}_i = S_i \tag{24}$$

- Drift-diffusion approximation

$$\boldsymbol{j}_i = \mu_i \; n_i \; \boldsymbol{E} - D_i \; \mathbf{grad} \; n_i \tag{25}$$

- Source terms for air:

$$\left\{ \begin{array}{lllll} \mathrm{S_e} & = & (\partial_t n_e)_{\mathrm{chem}} & = & (\nu_\alpha - \nu_\eta - \beta_{\mathrm{ep}} n_\mathrm{p})\, n_\mathrm{e} + \nu_{\mathrm{det}} n_\mathrm{n} + S_{ph} \;, \\ \mathrm{S_n} & = & (\partial_t n_n)_{\mathrm{chem}} & = & -\,(\nu_{\mathrm{det}} + \beta_{\mathrm{np}} n_\mathrm{p})\, n_\mathrm{n} + \nu_\eta n_\mathrm{e} \;, \\ \mathrm{S_p} & = & (\partial_t n_p)_{\mathrm{chem}} & = & -\,(\beta_{\mathrm{ep}} n_\mathrm{e} + \beta_{\mathrm{np}} n_\mathrm{n})\, n_\mathrm{p} + \nu_\alpha n_\mathrm{e} + S_{ph} \;. \end{array} \right. \tag{26}$$

- Local field approximation: $\nu_\alpha(|\vec{E}|/N)$, $\nu_\eta(|\vec{E}|/N)$, $\mu_i(|\vec{E}|/N)$, $D_i(|\vec{E}|/N)$
Morrow et al., *J.Phys. D:Appl. Phys.* **30**,(1997)
- Transport parameters and source terms are pre-calculated (Bolsig+ solver - http://www.bolsig.laplace.univ-tlse.fr/)

2D Fluid model for discharge in air at $\mathrm{P_{atm}}$

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2D Fluid model for discharge in air at $\mathrm{P_{atm}}$

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- Surface charges on the dielectric surface are obtained by time integrating charged particle fluxes to the surface.
- At the dielectric surface, secondary emission of electrons by ion bombardment

Specificities of the simulation of low-temperature plasmas at atmospheric pressure

- Simulation of ionization front propagation is known to be computationally **expensive**
- Temporal multiscale nature of **explicit** simulation: Δt=$10^{-12} - 10^{-14}$s

Convection: $\Delta t_c = \min \left[\frac{\Delta x_i}{v_{x(i,j)}}, \frac{\Delta r_j}{v_{r(i,j)}} \right]$ Diffusion: $\Delta t_d = \min \left[\frac{(\Delta x_i)^2}{D_{x(i,j)}}, \frac{(\Delta r_j)^2}{D_{r(i,j)}} \right]$

Chemistry: $\Delta t_l = \min \left[\frac{n_{k(i,j)}}{S_{k(i,j)}} \right]$ Diel. relaxation: $\Delta t_{Diel} = \min \left[\frac{\varepsilon_0}{q_e \mu_{e(i,j)} n_{e(i,j)}} \right]$

- Time scale of discharge propagation in centimeter gaps is $\sim$ 10 ns, $\rightarrow \sim 10^4$ time steps
- For a gap of 1 cm, Δx,r=10 $-$ 1 μm $\rightarrow$ nbre of points > 1×10^6

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<u>Convection:</u> $\Delta t_c = \min\left[\frac{\Delta x_i}{v x_{(i,j)}}, \frac{\Delta r_j}{v r_{(i,j)}}\right]$ <u>Diffusion:</u> $\Delta t_d = \min\left[\frac{(\Delta x_i)^2}{D x_{(i,j)}}, \frac{\left(\Delta r_j\right)^2}{D r_{(i,j)}}\right]$

<u>Chemistry:</u> $\Delta t_l = \min\left[\frac{n_{k(i,j)}}{S_{k(i,j)}}\right]$ <u>Diel. relaxation:</u> $\Delta t_{Diel} = \min\left[\frac{\varepsilon_0}{q_e \mu_{e(i,j)} n_{e(i,j)}}\right]$

- Time scale of discharge propagation in centimeter gaps is $\sim$ 10 ns, $\rightarrow \sim 10^4$ time steps
- For a gap of 1 cm, Δx,r=10 $-$ 1 μm $\rightarrow$ nbre of points > 1$\times$ 10^6

Specificities of the simulation of low-temperature plasmas at atmospheric pressure

- One time-step Δt: more than 50 % of the time for solving Poisson's equation
- Need for an accurate and efficient method to solve Poisson's equation at each time-step

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Numerical solution of Poisson's equation

$$Ve_{i,j}.V_{i+1,j} + Vw_{i,j}.V_{i-1,j} + Vn_{i,j}.V_{i,j+1} + Vs_{i,j}.V_{i,j-1} - Vc_{i,j}.V_{i,j} = -\rho_{i,j} \tag{28}$$

where

$$Vc_{i,j} = Ve_{i,j} + Vw_{i,j} + Vn_{i,j} + Vs_{i,j} \tag{29}$$

The coefficients Ve,Vw,Vn and Vs are known, the source term is also known.
We want to calculate $V_{i,j}$
$\rightarrow$ The system to be solved can be written as Ax=B.

Different methods can be used (iterative or direct methods).
In this work, we propose to use 2 iterative methods:

- Gauss-Seidel
- SOR (successive over-relaxation)

Numerical solution - Gauss-Seidel

$$Ve_{i,j}.V_{i+1,j} + Vw_{i,j}.V_{i-1,j} + Vn_{i,j}.V_{i,j+1} + Vs_{i,j}.V_{i,j-1} - Vc_{i,j}.V_{i,j} = -\rho_{i,j} \tag{30}$$

If we write the Gauss-Seidel algorithm, we have to calculate:

$$V_{i,j} = (-Ve_{i,j}.V_{i+1,j} - Vw_{i,j}.V_{i-1,j} - Vn_{i,j}.V_{i,j+1} - Vs_{i,j}.V_{i,j-1} + \rho_{i,j})/Vc_{i,j} \tag{31}$$

and iterate until convergence.

Numerical solution - successive over-relaxation (SOR)

The SOR method is a slight modification of the Gauss-Seidel method.

In the SOR, we define $0 < \omega < 2$ and calculate iteratively:

$$V_{i,j} = (1-\omega)V_{i,j}^{old} +$$

$$(-Ve_{i,j}.V_{i+1,j} - Vw_{i,j}.V_{i-1,j} - Vn_{i,j}.V_{i,j+1} - Vs_{i,j}.V_{i,j-1} + \rho_{i,j})\omega/Vc_{i,j} \tag{32}$$

until convergence

$V_{i,j}^{old}$ is the solution obtained at the last iteration.

If $\omega = 1$ we have the Gauss-Seidel method.

A good compromise for the SOR method is to use $\omega = 1.5$